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

PUBLIC MEETING MINUTES

JULY 7 - 8, 2015

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

July 7 - 8, 2015
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 7 - 8, 2015, 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	Persis Drell	Monica Olvera de la Cruz
Simon Bare	Roger French	Mark Ratner
William Barletta	Ernie Hall	Anthony Rollett
Gordon Brown	Sharon Hammes-Schiffer	Gary Rubloff
Sylvia Ceyer	Bruce Kay	Maria Santore
Beatriz Roldan Cuenya	Max Lagally	Matthew Tirrell
	William McCurdy, Jr.	John Tranquada

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

Committee Manager:
Katie Runkles, DOE BES

TUESDAY, JULY 7, 2015

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 Tuesday, July 7, 2015, at the Bethesda North Marriott Hotel and Conference Center by BESAC Chair **Dr. John Hemminger**. Committee members introduced themselves. Dr. Hemminger reviewed the agenda.

NEWS FROM THE OFFICE OF BASIC ENERGY SCIENCES

Dr. Harriet Kung, DOE, Director of BES, shared staffing changes to include the addition of **Katherine Chen** and **Thomas Russell** in the front office. New program managers are **Tom Settersten**, **Viviane Schwartz**, and **Chuck Peden**. There are two new interns supporting BES as well. **John Miller** will retire on July 23 and Kung thanked Miller for his service.

The Office of Science (SC) Early Career Research Program started in 2010. The first cohort was funded by the American Recovery and Reinvestment Act (ARRA). Eligibility requirements for the program have been maintained. Award length is five years. University recipients receive $150k per year, and national laboratory awards are a minimum of $500k per year. BES has made 158 awards out of a total of 356 awards given by SC over six years.

On average, Early Career Research Program award recipients are 5.5 years out from receiving their PhD. The number of proposals has decreased since program initiation in 2010. Twenty-five awards were made in 2015. The average proposal success rate is 4.8 percent.

Kung highlighted the work of Early Career Research Program award recipient Athena Safa-Sefat at Oak Ridge National Laboratory whose research combines material discovery with theory and advanced characterization. Safa-Sefat is among the top one percent of highly cited researchers and is a good example of the awardees. Martin Centurion is another recipient, studying ultrafast electron diffraction at the University of Nebraska, Lincoln. Centurion is a key contributor to the development of and first images with SLAC National Accelerator Laboratory's MeV ulftrafast gas-phase electron diffraction capability. Volker Rose is a 2012 award recipient at Argonne National Laboratory. He is combining scanning probe microscopy and synchrotron radiation for nanoscale imaging with chemical, electrical and magnetic contrast. Rose received a patent for a way to simultaneously determine physical structure and the chemical make-up of materials close to the atomic level.

The National Synchrotron Light Source-II (NSLS-II) first achieved light on October 23, 2014, and reached project completion in March 2015. Latest results include the storage of 250 mA in the storage ring in June 2015. There have been exciting results since early commissioning.

A briefing was held at the U.S. Capitol Visitors Center on June 25, 2015 to highlight the contributions of DOE's light sources. The event was co-sponsored by the Senate National Laboratory Caucus and the House Science and National Laboratory Caucus. An industry representative panel shared diverse testimonies. Dow Chemical highlighted the use of light sources to look at very fine details of carbon fiber structures, the distribution of fibers, and the use of 3D imaging to look at parts fabricated using polymer sources. Toyota North America uses light sources to examine chemical reactions occurring in rechargeable magnesium battery technologies. Intel Corporation is using light source capabilities to expand the capabilities and potential of computer chips. Pharmaceutical makers use light sources to develop new drugs and advance pharmaceutical capabilities for public impact. The event included the release of a website that describes detailed SC user statistics from across the range of facilities that SC supports, to include the light sources.

BES looked at a case study of the evolution of solar research cell efficiencies. The work reflects huge global investments. There are clear linkages to long term basic research support. In multi-junction GaAs cells, primarily supported at the National Renewable Energy Laboratory (NREL), researchers correlated the defect structure to the electronic properties. At the Light-Material Interactions in Energy Conversion Energy Frontier Research Center (EFRC), a photon recycling scheme has allowed for the creation of a device with increased light absorption. Work at NREL put multi-exciton generation on the map and is another example of an emerging technology. Collectively over a decade, there is clear impact due to investments and the transfer of knowledge through publications leading to significant scientific advances.

The lithium-ion battery has evolved along with increased energy density and decreased cost. Near the mid-1990s, lithium ion battery use started to grow and new types of cathode materials were discovered. An example is lithium iron phosphate, with research being done at MIT and Argonne that draws on BES support. The work at Argonne started in the mid-1990s. Concerns over safety and performance drove the study new cathode materials. Argonne's work is being used by General Motors. This is a success story with clear lineage to BES support.

Another example of effective BES support is solid-state lighting. There has been impressive growth, especially since the first visible deep red LED was not discovered until 1962 and LED as a lighting option was not possible until the development of blue LEDs in Japan in the late 1980s. When combined with other LEDs, this can produce the white LED technology being used today. Advances relied on fundamental physics research at Sandia National Laboratories (SNL) and BES support. SNL has developed *in-situ* diagnostics to monitor growth of the buffer layers and link to modeling tools.The technology has transferred to commercial use and the *in-situ* monitoring of semiconductor layers is now being done.

BES support for nanoscale science embodies another example of scientific advancement. Display technologies use quantum dots discovered through BES-funded research.

These examples show the impact of BES research and how it can drive new directions. BES looks forward to the report out from BESAC to identify exciting new directions.

The FY16 BES budget request totals $1,849M and is a $116M increase from FY15. The House and Senate appropriation marks for BES differ. The House mark is $37M more than the FY15 appropriation, while the Senate mark is an $111M increase over FY15. These are good marks considering that SC overall is relatively flat.

The House mark provides $97.8M for the EFRC portfolio but is a cut compared with FY15. Computational Material Sciences will stay flat. The hubs are at the requested level. User facilities are lower than the request, but APS-U and NEXT are funded at the request level. For LCLS-II, the House recommends $191.9M which is $53M above FY15.

The Senate mark is $5M below the request. There are specific numbers for the neutron and light sources and $125 M for NSLS-II, which is $15.5M above the request. The Senate language requested that BESAC take on a study to prioritize the next five upgrades and major construction projects and deliver the report no more than 90 days after the enactment of the act. The Senate recommended $3M for a competitive solicitation for universities to develop a new generation of nanostructured catalysts that can be used to synthesize fertilizer and ammonia with any secondary greenhouse gases.

The current charge presented to BESAC calls for an evaluation of the breakthrough potential of current and future energy science frontiers based on how well the research advances the five grand science challenges. Studies since 1999 have allowed BES to grow its portfolio, and this speaks to the credibility and authority of BESAC.

BES will hold a Basic Research Needs workshop for Environmental Management on July 8 – 10, 2015. The workshop is co-sponsored by the Offices of Biological and Environmental Research and Advanced Scientific Computing Research.

Kung highlighted efforts to communicate BES research, including the new "Nanotechnology: Energizing our Future" placemat.

Discussion

Hemminger asked if there are any statistics on follow-on success from the early career program. **Kung** shared the SC is constructing metrics that will assess achievements starting with the first cohort which is about to graduate from the program.

Simon Bare asked about the House and Senate marks. **Kung** noted that occasionally there has been such directive language, and that this year's language was somewhat unusual. **Hemminger** asked whether no new EFRC solicitation in FY16 is a foregone conclusion at this point. **Kung** replied that the Senate was silent on the funding for EFRCs, so BES has flexibility if we cut the core program. However, BES is not contemplating this. BES does want to start the EFRC solicitation on an biannual basis.

Bare asked about statistics for specific subject areas. **Kung** shared that BES does have those numbers and will discuss sharing those numbers with the community.

UPDATE ON REPORT BY THE BESAC SUBCOMMITTEE ON TRANSFORMATIONAL OPPORTUNITIES

John Sarrao shared an update on the draft report, "Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science." The subcommittee is still integrating input from BESAC members.

The report has evolved since the February 2015 BESAC meeting to point out transformative opportunities and elements to enabling success. There are five opportunities that are the basis for the report. These are distinct from the grand challenges but also build on the challenges. There are multiple themes in the report that need tightening and mechanics that need to be addressed.

The message of the report draws on discussions held since 2007. At the time, basic research needs workshops helped identify specific and broad themes. The EFRCs and the early career program did not exist, and there were many open questions that were presented. Since 2007, the portfolio has been shaped to move the field in ways that are very compelling. Facilities and other means to accomplish research have been started and grown.

The original 2007 Grand Challenges report proposed questions that are still compelling. The new report points out that there is significance and value in addressing these questions, and there are opportunities to accelerate how those questions are addressed. The new report will distill the questions and demonstrate deep and exciting opportunities to address those questions.

Three opportunities addressed in the report are:

- Mastering hierarchical architectures and beyond-equilibrium matter
- Beyond ideal materials and systems: Understanding the critical roles of heterogeneity, interfaces and disorder
- Harnessing coherence in light and matter

Two cross-cutting opportunities addressed are:

- Revolutionary advances in models, mathematics, algorithms, data and computing
- Exploiting transformative advances in imaging capabilities across multiple scales

These are the core of the report, and will allow for the kinds of changes over the next decade that have been seen since the 2007 report.

Sarrao explained that within "mastering hierarchical architectures" there are new ways to manipulate matter and the potential for targeted functionality in materials by controlling the synthesis and assembly of hierarchical architectures beyond-equilibrium matter. This opens a wide opportunity space.

"Beyond ideal material and systems" shows that this is not the first time researchers have thought that not all materials are perfect. As it relates to opportunities at the mesoscale, imperfections are quite good and actionable. Considerations to be made include how manipulation and control plays a role in thinking about scale, and how to consider events, epidemiological studies, degradation and lifetime predictions.

"Harnessing coherence in light and matter" is of a dual nature. This is being actively exploited, but it is a scientific frontier unto itself. The extent to which the evidence of coherence is appreciated will point to a broad frontier space going forward.

The cross-cutting theme of "models, mathematics, algorithms, data and computing" will accelerate progress on the grand challenges.

“Exploiting transformative advances” and the synergy between data and imaging. Research needs to consider if this can be done in a multimodal way that will allow for measuring phenomena that are complex and important for fundamental science.

Getting from here to the future means acknowledging that past research embraced opportunities like the EFRCs and the early career program. The domain for future opportunities includes synthesis, advancing instrumentation and tools, and raising a new generation of scientists and guiding current scientists as stewards of the growing workforce.

In the area of synthesis, research can embrace opportunities like materials science, materials genomics, and predictive inverse design. Significant investment is needed. It is recommended that BES lead the way in embracing computational materials science and advanced synthetic approaches. Their integration is a critical initiative.

Within instrumentation and tools, new capabilities yield new insights. BES should empower investigators skilled in instrument development and consider the skills needed for future scientists.

In the area of workforce, the key word is balance. BES has a robust and exciting portfolio. A key consideration to be made is how to bring together the gains of capabilities such as in the EFRCs and maintain that balance while building scientists’ skills and ensuring a balanced portfolio of core investments. Strengthening connections and fostering the next generation of energy scientists are also important.

The report will show that the grand challenges are still compelling and exciting, and can be accelerated. There are also new opportunities that can be advanced through specific investment.

REPORT ON THE QUADRENNIAL TECHNOLOGY REVIEW

Dr. Lynn Orr, Under Secretary for Science and Energy, DOE, highlighted changes occurring in energy use and technology in the energy landscape. The U.S. energy landscape is undergoing dramatic change, and it will be strengthened through changes in the science.

The Obama Administration’s 2013 Climate Action Plan prioritized a reduction in carbon emissions, preparation for the impacts of climate change, and the development of international efforts to address global climate change. In November 2014, the US made a historic commitment to reduce greenhouse gas emissions by 26 to 28 percent below 2005 levels by 2025.

The DOE has two studies underway. One is the Quadrennial Energy Review (QER) focused on the energy infrastructure of the U.S. There are recommendations to support that review. The Quadrennial Technology Review (QTR) aims to take a snapshot of the status of energy technologies and identify opportunities for additional progress. The latter recognizes the value of the underlying science needed.

The process being used to assemble the QTR includes technology assessments that analyze the current status and opportunities of individual energy technologies by sector.

A series of workshops lead by the DOE and an external peer review have guided the accuracy of the QTR. The review serves as an educational guide describing the status of various technologies. Six sectors and systems analyses are described in the QTR, each highlighting specific areas of technology.

The QTR combines applications and research, and enables the identification of productive links across programs. Detailed conversations across the whole agency and with the national laboratories are producing benefits and have informed the QTR

The modern grid is a fundamental element of modern societies. The current grid was designed a century ago. It is driven by regional operators and is characterized by turning on and off power plants, and thus a slow pace in estimating needs and deciding what to do. There is a tremendous need for sensors and data acquisition, and thinking about physical and cybersecurity concerns that will control the reliability of the grid going forward. Thinking about this will result in a more reliable grid with greater ability to prevent outages and provide power.

The clean electric power system is coming about due to the impending rules under the Clear Power Plan. This area holds great potential for carbon capture. There is more work to be done in the separation side, in particular. The key conclusion is that having a well-diversified power generation system is of huge benefit. The ability to manage the variability of various sources is important.

Around 40 percent of U.S. energy use is in buildings. A building is a fairly complex system due to thermal comfort, lighting, and plug loads. The systems level of building management is just being understood as are ways to capture waste and turn it into services. There are opportunities in electrical power distribution especially related to systems interfacing with systems.

In the advanced manufacturing area, there is a wide range of potential applications. Each offers something that can have a real impact. DOE is looking for places where there is opportunity for impact by totaling up all energy-using activities and looking for those using on order of one percent of all U.S. energy.

In the cleaner fuels side, the oil and gas area is well-researched but there are significant environmental impacts to be addressed. Within bioenergy, DOE is very active and there are many opportunities in the gathering and conversion of energy stored as chemical bonds into something like fuel or an energy service. And in hydrogen, there are gains to be made on a large industrial scale, but it is currently mostly made from natural gas reforming. DOE is looking at other ways to generate hydrogen as one way to reduce gas emissions.

SC is fundamentally enabling all of these activities by funding underlying work. That needs to be covered in the QTR. The x-ray light sources, neutron sources, and the Nanoscale Science Research Centers are all aimed at understanding the fundamentals of how novel materials can be put to work in energy applications.

Exascale computing is a major effort in the DOE. Understanding fundamental physics and chemistry at a point where the prediction of materials and ways in which they operate would help close the design loop and speed the integration of materials into applications.

There has been a lot of experimentation at DOE. Teams are working on hard problems that matter for the future. The EFRCs, the Energy Innovation Hubs, and the Bioenergy Research Centers are examples of efforts to drive better understanding of fundamentals and drive innovation.

DOE has supported collaboration and cross-fertilization of HQ and National Laboratories through budget cross-cutting initiatives such as grid modernization. DOE is also forming technology teams to address issues such as clean energy manufacturing.

The QTR is nearing completion and should be available soon.

Discussion

Bill Barletta suggested a focus on advanced materials research to advance the lifetime of nuclear plants. **Orr** confirmed that this is included and it is fundamentally a materials issue. We need to better understand materials that are in high-radiation and high-stress environments.

Orr responded to **Monica Olvera de la Cruz**'s interest in knowing whether solar energy was covered. The deployment side is very active and solar panel costs have come down. Balance of plant costs are higher than panel costs and there is clear opportunity from the study for transforming multiple photons into electrons. That is a material issue and one where there is thermodynamic headroom.

Bill McCurdy asked about balancing resources and activities in the context of the QTR, noting that natural gas production seems economically feasible yet political discussions focus on activities such as solar energy. **Orr** agreed that the QTR spans the spectrum of opportunities and that there are roles to be played by DOE and industry. A fully diverse research portfolio would be distributed along timescales and not react slowly to short-term price swings in commodity markets. The energy mix will evolve. DOE can provide tools across that spectrum and reduce cost projections to allow for competition in a broad way.

Tony Rollett noted the value of a historical perspective on how energy technologies come and go, and yet the timescale for fundamental research is much longer. **Orr** suggested that the QTR is lengthy but could have more of a long-term historical view. That view is valuable and wrapped in the discussion of how innovation occurs. The idea of providing a commercial activity is the weaving of many threads, some of which are ready at different times. Research can weave those threads and help to see future threads not yet clearly visible. Telling stories is a useful way to enable public understanding about energy and specific projects at DOE facilities.

Hemminger noted that computational power advances and the maturity of underlying theory empower complex systems modeling. **Orr** agreed that mathematical underpinnings are part of current and future challenges. Even with exascale computing, work is needed on the software and mathematical sides. The absence of physical testing of nuclear weapons called for advanced computing. The rest of the scientific community recognized other applications. Once the community can address the multi-scale challenges before us, it will open up a whole new opportunity space.

Beatriz Roldan Cuenya noted an emphasis by some on new construction over projects and operations funding. **Orr** shared that the DOE recognizes the need to balance construction and operation funds. SC colleagues are thinking through this balance.

NEWS FROM THE DOE OFFICE OF SCIENCE

Dr. Pat Dehmer, Acting Director, Office of Science, shared insights on program planning, the role of advisory committees, and advances made by the six SC divisions.

The SC FY16 President’s Request is $5,340M. The BES request is $1,849M and the House and Senate marks for BES differ based on different priorities. Significant differences for SC are decreases in support from the House for Advanced Scientific Computing Research (ASCR) and lower marks from the Senate for Fusion Energy Science (FES). SC is waiting for conferences in the fall of 2015.

The Office of the Under Secretary for Science and Energy is responsible for 13 DOE laboratories. The Office consists of seven offices to include the SC. In April, senior laboratory leadership visited DOE to share their annual strategic plans.

Within the SC, about 93 percent of funds flow through the offices and out to the performers. About four percent goes toward safeguards and security and small construction projects at the labs, and the remaining three percent goes toward salaries and the SC workforce.

About 73 percent of funding in FY14 went to the 10 SC national laboratories, 16 percent went to universities, and about six percent went to industry. In FY15 about 42 percent of the funding was committed to research, 39 percent to facility operations, 13 percent to projects, and six percent to other needs.

SC program planning is driven by mission need and scientific opportunity. SC's mission needs are top-down directionfrom the Executive branch and Congressional branch. SC's scientific opportunities are bottom-up priorities from community and stakeholder engagement. This is also where Federal Advisory Committees such as BESAC play an important role. Nearly all major SC facilities and research programs are rooted in federal advisory committee reports and recommendations.

Major SC program funding from 1978 through 2015 has fluctuated. Growth in BES has occurred through the creation of new facilities, new scientific opportunities, and the Quadrennial Technology and Energy Reviews. BES has grown from less than 20 percent of the SC budget to nearly 40 percent in FY15. Fusion Energy Sciences started as a high percent of the SC budget and has since leveled off, despite investing in facilities in Europe. High Energy Physics was a large program in 1978 and grew to its high point in the early 1990s due to the Superconducting Super Collider, It is now at its lowest point in many decades. Nuclear Physics has stayed at around 10 percent.

The Advanced Scientific Computing Advisory Committee (ASCAC) has focused on data-intensive science and exascale computing. It identified 10 principle research challenges and technical approaches to develop exascale computing systems, and reviewed preliminary conceptual designs for the Exascale Computing Initiative. ASCAC engages industry to improve computing power while drawing fewer energy resources. Over the lifetime of this work, the budget is in the billion dollar budget range.

BESAC provided guidance on photon sources and science, and is currently considering new science opportunities. The BESAC report on Future X-ray Light Sources brought about dramatic change and is an example to other committees on the impact of reports. Like ASCAC computing activities, these activities are in the billion dollar range. The current revisiting of the 2007 Grand Challenges Report will likely be another impactful report.

The Biological and Environmental Research Advisory Committee (BERAC) is currently considering initiatives for field-based research to capture multi-disciplinary approaches and build on observations and modeling. It has defined criteria for selecting sites for future field-based research and identified ways to prioritize the sites identified. BERAC was charged with this in 2014 with a final report due in Fall 2015.

The Fusion Energy Science Advisory Committee (FESAC) has focused on strategic planning for fusion energy sciences in responses to a charge from Congress. FESAC was also asked to assess connections between research supported by the Fusion Energy Sciences program and other scientific disciplines and technological applications.

The High Energy Physics Advisory Panel (HEPAP), through the P5 panel, developed a strategic plan. The report identified five scientific drivers. BESAC's draft echoes this successful report. HEPAP's recommendations include forming an international collaboration to build a long baseline neutrino facility to be hosted by the U.S. SC expected that it would take a minimum of two years to develop these partnerships but they are already being lined up. The second HEPAP charge is to assess the accelerator R&D effort supported by High Energy Physics.

The Nuclear Science Advisory Committee (NSAC) is guiding the creation of a possible second generation U.S. experiment on neutrinoless double beta decay capable of reaching the sensitivity needed to determine if the neutron is a Majorana or Dirac particle. The NSAC is also conducting a new study of the opportunities and priorities for U.S. nuclear physics research. It will recommend a long-range plan that will give a framework for the coordinated advancement of nuclear science research programs over the next decade.

When planning annual budgets, SC looks out over five years and beyond. One driver is investing in exascale computing. Another is BES light sources as recommended by the light source report. The other is the hosting of an international neutrino facility in the U.S..

BESAC could invite speakers from other committees to learn how their committees work.

The QTR has been briefed to the DOE Secretary. SC briefed OMB on chapter nine. A number of OMB examiners and senior management were in attendance. Dehmer was asked many questions, specifically related to the 2007 grand challenge report and the specific accomplishments that had taken place. OMB has asked to be briefed on the next BESAC report.

Discussion

Rollett asked what lies behind the House and Senate committees' varying priorities. **Dehmer** shared that each committee has a bottom line and priorities to address. Often, the staff who do the marks are reflecting the priorities of one or two members of the committees.

McCurdy indicated that there seems to be an imbalance between materials and chemical sciences in BESAC's draft report. **Dehmer** responded that the last two opportunities in the report are tools and the first three are scientific challenges. HEPAP's report as an example had broad science challenges that were balanced across the program. BESAC's draft discussed the three broad areas. She wondered about weaving in the core research activities as underlying elements. Authors could consider others' interpretations and think about how core programs will contribute to these challenges.

Hemminger noted that BESAC differs from other committees in that it provides advice to BES and SC but has not told BES what to do. HEPAP may give direction to High Energy Physics. BESAC's report may differ in that it presents opportunities. **Persis Drell** added that a past challenge for HEP was the community's balkanization. BESAC's report describes scientific challenges and is not a long laundry list. **Dehmer** commented that the HEP P5 panel was originally formed to look at projects. The Nuclear Science Advisory Committee started in the same way, and looked at various budget scenarios. Congress directed FES to do a strategic plan. It drives the results in a way that is usually not optimal. The remaining programs have not done that and have better results. BESAC has taken on the hard task of looking at projects and deliberately stayed away from the minutia.

McCurdy suggested that the draft does not represent academic disciplines in the same way that the 2007 report did. He wants to avoid the idea of developing a laundry list.

Hemminger asked about exascale computing and how that technology will address scientific problems. **Dehmer** shared that SC is thinking about ways to work with computers that are more and more powerful. The second big part of SC's investment strategy is to draw on experts who can develop codes for exascale computing.

Barletta asked about FES investment in plasma science. **Dehmer** shared that plasma science is a small fraction of FES and is hurt due to cuts. There are few agencies that contribute to plasma science. It should be a stewardship issue for SC.

REPORT ON THE FY15 COMMITTEE OF VISITORS BES DIVISION OF MATERIALS SCIENCES AND ENGINEERING

Gary Rubloff, Chair of the FY15 Committee of Visitors (COV) for the BES Division of Materials Sciences and Engineering (DMSE), shared the results of the COV conducted on March 10–12, 2015. The COV responded to a charge to examine processes used to making funding decisions for proposals and the DMSE's ability to deliver world-class science.

The COV of 15 panelists in four panels found that DMSE effectively manages a world-class portfolio whose dedicated leadership teams are engaged with the community. Leadership teams listen to the community and make decisions based on priority areas, allowing them to effectively evolve their portfolios. The PAMS tool was effective in enabling the COV activity.

DMSE supports an exceptional core research program even as its scope expands. It is challenged by travel funds reductions that limit interaction between PIs and the community.

One recommendation is that core programs should receive new funds to execute opportunities that will be identified in the BESAC update to the 2007 Grand Challenges report. The COV recommended increased travel funds.

The continued use of white papers was recommended to help guide program managers' advice to PIs before and after the paper submissions. Program managers can give timely, informal, frank and detailed guidance to PIs before and just after white paper submissions.

Research highlights assembled in PowerPoint and Web format are a valuable synopsis of the portfolio and help to communicate its value to a broad audience

The COV recommended continuing the biennial meetings for PIs and program managers.

Research emphases and de-emphasis are shared with the community, but should be more systematic.

The COV recommended maintaining the balance among the three EPSCoR funding modes: implementation grants, laboratory partnership grants, and early career awards.

The COV found that the membership size of 15 was good. Summary reports from the panels were included in the report. **Rubloff** commented that research highlights should be read by the COV members in advance of conducting the portfolio evaluation.

Discussion

Gordon Brown shared that the burden of decreased travel costs came up nine years ago during a chemistry COV. **Kung** noted that since the DMSE COV, the BES has received an additional $55k in travel funds and foresees that BES can plan better in the next FY for this need. **Dehmer** added that SC looked across the office to assess travel budget levels and found that some associate directors had travel funding per traveler at levels much below others. BES was one of those offices. SC wants to set a new base to ensure equitable funding across the offices and increase travel funds, despite the burden of Congressionally-imposed travel restrictions in 2010.

Sylvia Ceyer asked about the proposal success rate. **Linda Horton** shared that proposals were presented to the COVs on a core research activity level. BES is looking at the full funding of grants. Analysis shows that the success rate has not dropped to one-third, but there was still an unavoidable impact due to budget levels.

Ernie Hall participated in the COV and suggested that this size could be a model going forward.

Bare noted a recommendation that support should be given for the skills mix required to prepare the research highlights. **Rubloff** clarified that there is a need for those with a technical background to describe the research highlights to those on the Hill and other groups and show the accomplishments to broad audiences. Some people at BES are good at graphics, writing and public relations, and that is vital. **Horton** pointed out that current intern **Ashley Dyke** is an English major and helps with writing. **Kelly Perry** is on detail from Oak Ridge to help manage science programs and manage the message and convey highlights. This reduces the burden on programs managers, too.

Max Lagally moved to approve the report, and the BESAC unanimously approved it. The report will be formally transmitted to Dehmer. The cover letter will highlight travel with an emphasis on communicating research highlights and the update to the Grand Challenges Report. **Dehmer** asked that the cover letter highlight the value of PAMS.

UPDATE ON THE LINAC COHERENT LIGHT SOURCE-II

John Galayda shared that the Linac Coherent Light Source (LCLS) took 17 years from idea to first light in 2009. BESAC played an important role in bringing attention to focused lasers, and can be seen as far back as a report from BESAC in 1997.

LCLS uses the last third of the existing linac tunnel and was a multi-laboratory project. The facility has produced higher energy pulses and pulse durations beyond initial projections.

The facility draws 600 users per year and 138 high-impact papers have been published to date.

New operating modes have been implemented at LCLS. These include controllable polarization and the ability to produce two color operations. Single shot crystallography is now possible.

There is competition from the SACLA facility in Japan. Facilities are also planned in Europe and Korea.

LCLS results prompted discussions of an upgrade to LCLS-II. This started in 2009. Options considered included using the existing SLAC Linac. BESAC's 2013 report impacted discussions. It recommended a high repetition rate and greater pulse characteristics needed for a broad range of pump probe experiments. This provoked the need for a superconducting linac at 4 GeV. The upgrade includes two undulators to get the spectral cover desired. Existing instruments will need to repurposed to exploit the capabilities of both sources.

The copper linac in the first kilometer will be replaced by a 700m superconducting linac. The middle linac already in existence will stay intact, and electrons will be transported past this linac in a separate channel.

The superconducting linac requires 35 superconducting acceleration modules and two higher-frequency modules. The design is based on module designs from the ILC and European XFEL.

The design goals are for high average brightness, based on the production of 20W average x-ray power. Once achieved, this level will be world-leading in brightness.

This change in project configuration drew upon collaboration between Fermilab, Jefferson, Berkeley, and Argonne National Laboraties and Cornell University. Each are providing specific equipment for the new design and will contribute to the R&D and planning phases.

The full project baseline is slated for FY 2016. The proposed CD-4 date is 2022. Progress is possible through using designs and equipment developed for other facilities, leveraging ongoing R&D and operational experience from the creation of LCLS, and using existing infrastructure.

The gun to be used has a frequency of 186 MHz. The accelerating structures are made of nine-cell niobium cavities put in a helium jacket. These cavities will undergo nitrogen doping to increase Q. The higher the Q, the lower the power bill, and possibly the higher the gradient. The doping process is being transferred to industry. This is the first time that doping will be exploited in a running linac.

The LCLS-II cryomodule is very similar to the ILC/XFEL cryomodule. It fits in the SLAC tunnel.

The refrigeration of systems makes use of an existing Jefferson Laboratory design.

An LCLS-II workshop held in February 2015 discussed the science opportunities for LCLS-II. There are many capabilities; hence instruments need reconfiguration to match this realm of techniques. Longer term opportunities requiring R&D include 10x to 100x increases in peak power, control of electron beam properties on a micron scale, and the controlled modulation of color, amplitude and phase of x-ray pulse.

The LCLS-II design has been responsive to BESAC report recommendations, is moving quickly due to partner laboratories, and has advanced due to ongoing accelerator R&D efforts.

Discussion

Galayda shared with **Hemminger** that a leading item in the establishment of the LCLS-II is fulfilling the refrigeration plant. The cryoplant acquisition process takes three years. The cryomodules are another big driver in the upgrade timeline. There have been unexpected delays with some vendors which may dictate the timeline. LCLS will need to be turned off to take apart the front ends and replace the undulators to accommodate the upgrade.

UPDATE ON THE ADVANCED PHOTON SOURCE UPGRADE

Peter Littlewood described the Advanced Photon Source Upgrade (APS-U) and a response to BESAC's report from July 2013 to move forward with the diffraction-limited storage ring upgrade to ensure that the U.S. retains its global leadership position in storage ring x-ray sources.

The APS is 20 years old. Improvements in storage ring capabilities have grown and there is growing global competition from Brazil, China, Japan and other countries.

The Upgrade will be a next-generation x-ray synchrotron. Optics, detectors, simulation and computing all have to be considered to make the machine as useful as possible. The current machine will be upgraded to 6 GeV and 200 mA. The current tunnel will emptied and filled with a multi-bend achromat lattice.

The APS-U is a high energy machine that will allow for penetrating experiments in bulk. It will be two to three times brighter, allowing for better resolution, wide fields of view, and imaging across scales. It will feature fast sampling with chemical, magnetic and electronic sensitivity. The use of coherence will allow for high spatial resolution even in non-periodic materials. Correlation methods will improve by 10,000 to 1,000,000 times.

The community has identified potential early experiments. Six workshops invited researchers to share diverse views. Themes that have emerged include imaging heterogeneity and the goal of unifying aspects of diffraction and imaging. Other themes are the ability to probe across length and time scales, non-equilibrium structures, and unraveling transport in complex systems to understand chemistry.

The Upgrade will give unprecedented opportunity for 3D atomic reconstructions. Amorphous metals can have high strength but can be very brittle. The upgrade will allow experiments to understand defects in unordered materials.

The Upgrade will also allow for looking for new zeolites which could be important for catalysis, fine chemicals and gas separations. There are about 200 known zeolites but potentially many more. X-ray fluctuation microscopy can probe ordering from sub-nm to microns during assembly from precursors to an ordered unit.

Big data management and computational capabilities are needed to manage APS-U discoveries. The integration of computational methods is an important goal.

The Upgrade is ideally suited to meet challenges identified in the upcoming BESAC report.

Littlewood described the physical changes that will need to occur. Equipment in the current ring will be replaced. The priority for the beamlines is to take advantage of the leap in source performance. A call for beamline proposals will be announced following CD-1, expected in September 2015. Some areas for experimentation have been identified. When the LCLS-II is turned on, it aims to have the highest performing suite of beamlines.

The global landscape has been helpful in providing some lessons learned for the Upgrade. Between now and 2022, there are new machines and upgrades expected in six countries.

The project plan features a conceptual design that is now complete. There have been many technical reviews that have examined and validated the design and scope. The APS-U will involve a 12-month downtime for removal, installation and testing.

CD-1 is expected in September 2015, with CD-2 in early FY 2017, CD-3 in early FY 2018, and CD-4 at the end of FY 2023.

Discussion

Littlewood confirmed for **De la Cruz** that the project plans for the magnets to be assembled in sections at Argonne and then installed in the tunnel. There are 3,000 tons of magnets. There are five entry points into the tunnel to allow for work to be done as quickly as possible.

Littlewood shared with **Ceunya** that the beamlines and everything will be switched off during the downtime. Some of the beamlines would be upgraded before the shutdown and others when the ring is being installed so that they are all available for operations when installations are complete. The facility will operate more than 60 beamlines. APS is conscious of having 5,500 users hence it cannot afford to bring the machine back up with only half the beamlines.

Littlewood clarified for **Cuenya** that there will be separate work done on detectors as this is usually part of the operations budget. This discussion is still open.

Drell asked if there will be any collaborations with other laboratories. **Littlewood** shared that just one institution does not have the ability to run this and do everything that is desired. There is a lot of expertise at other laboratories. There needs to be a greater sense of the scope and then there will be more formal discussions.

Barletta asked about plans to include unusual pulse modes for users such as compressed bunch modes. **Littlewood** noted that multiple bunch modes are being considered. They are using two bunch modes as a benchmark and there could be others to consider. APS would like engagement from the community on issues such as this. The community has not quite self-organized yet and the APS does not want to rule things out because it failed to identify them.

Littlewood clarified for **Hall** that there is discussion going on with partners about how to use their beamlines. Partners will have the opportunity to upgrade those beamlines within the schedule.

DISCUSSION OF THE BESAC CHALLENGES REPORT

Hemminger invited comments on the “Challenges at the Frontiers of Matter and Energy: Transformative Opportunities for Discovery Science” draft report. The goal is to have the report in production at Argonne by the end of July.

McCurdy noted that chapter two talks about mastering hierarchical architectures and yet the examples shown do not relate to the challenges of synthesis or related chemical aspects. There are many examples that could be shown here. As written, the chapter does not allow chemists to see themselves in that section.

McCurdy added that the section on coherence is a descendant of discussions in the 2007 report. This unchained a whole range of research in chemical science and in DOE that made use of the justification for LCLS-II. The molecular examples shown in this section do not relate to this, and that community may not see itself here.

McCurdy reflected on the theory section, noting that in the past 20 years, the chemical theory community has moved to larger and more coherent systems and excited states. That community may not see itself in that section and there are not any related examples. Opportunities should be identified and give all communities a presence in the report.

McCurdy suggested that material science and chemistry is so interconnected that it is harder to see the separation. There are many ideas that come to mind but no examples in the report.

Sarrao acknowledged the details provided by **McCurdy**. **Hemminger** asked **Matthew Tirrell** if a chemist would see oneself in chapter two. **Tirrell** commented that the elements cited by **McCurdy** are true. Improvements could be made in the draft if there is a focus on chemical reactions and catalysis. However, the section broadly addresses big challenges. **Hemminger** urged the need for the next draft to allow people to see themselves and their work in the content.

Rollett reflected on **McCurdy's** comments, expressing worry that most of the examples would be about materials. More or alternate examples could reflect catalysis and other themes.

Rubloff offered that the first two paragraphs of the Executive Summary are exciting. The third paragraph, however, gives examples for future work that seem clumsy and are enablers that many not be relatable for a lay reader. **Sarrao** agreed and shared that there edits to this section. **Hemminger** added that discussions have been had about "why now?" and that the answers need to cite advances in science and not just the value of better machines.

Cuenya added that there could be more examples about catalysis. **Hemminger** suggested that this could be addressed by an example from **Bare**.

Rollett noted that the report on mesoscale science could be borrowed to explain why there are new opportunities. **Sarrao** added that there could be too many examples in the report but agreed that the mesoscale report could be useful.

Ceyer added that some of the scientific accomplishments are in the appendix and don't have good coupling to the sidebars in the introduction. The grand challenge sidebars are helpful, but a sentence could be added that references the appendix. **Sarrao** agreed that that could be done.

Hall added that the report is well organized and that the five opportunities are the right ones. He was derailed by the first two opportunities in the Executive Summary as the examples do not tie in with "why now?" and "why this?" Well-known examples such as 3D printing could be more relevant and understandable. The last three opportunities are well-stated.

Drell highlighted the emphasis on the science opportunities and a need to call out DOE's impressive facilities as a foundation. A staffer who is guiding multi-million dollar support for facilities might come away perturbed. **Sarrao** shared that the examples that are sidebars were carefully chosen to be a balance between university and laboratory examples. A knowledgeable reader would know which is which but the use of the large facilities could be made clearer. **Drell** offered that the science being done is done at world-leading facilities and this could be noted in the introduction. **Hemminger** commented on the need to not emphasize the facilities over scientific achievements. The BESAC report on light sources described the value of the facilities but may not be remembered, so a statement in the beginning about this report may be useful.

Barletta noted that chapter six described how instrumentation being used at facilities is finding things never seen before and in new ways. That could be stated upfront. **Sarrao**

commented that the majority of the content is looking good but the opening needs another review.

Rollett added that facilities are mentioned in chapter six but perhaps do not come through as strongly. **Drell** commented that there is a sentence about facilities in chapter six that could be at the front. **Sarrao** added that showing this on page 41 may be too far back in the report.

Lagally noted that there are some things that do not come through clearly. One example is saying that we always work on equilibrium matter as that is not true. Much of the work done in the past 30 to 40 years has dealt with interfaces, yet it is described in the report as being entirely new. He added that chapter two seems to have been written by chemists and care is needed to manage the backgrounds of those writing the report. **Sarrao** noted that there are gaps that need to be addressed. **Hemminger** clarified that **Lagally's** first comments refer to the relatively loose prose in the opening section.

Rubloff added that keeping track of the logic in the report is critical. There were transformative things that emerged from 2007 and advances have been made. Chapter one of this report could describe that progression, and note that new progress is based on past success. **Hemminger** added that in the past, BESAC has produced a shorter report and a longer, more descriptive report. If the executive summary is done correctly, it can address that. **Sarrao** added that every chapter has a framing quotation but the executive summary does not. The white space shown in the executive summary could feature the five opportunities.

Bare commented that the title of the report conveys the matter theme but energy does not come out strongly, and challenges and opportunities described by DOE and **Orr** do not come across. **Sarrao** pointed out that responding to the "why now?" question could bring up energy.

McCurdy commented that the cover is nice. **Sarrao** shared that the cover is based on a scientific result. He welcomed feedback on the cover.

Ceyer commented that if the group decides to use the tree graphic, she would like to see the enablers as something other than clouds.

Hemminger acknowledged that very specific feedback has been received and asked if the BESAC is ready to accept the report with the understanding that notes that have been taken will be incorporated into the report. **Sarrao** added that this will include the detailed comments that have been received in the last week. **Lagally** offered to help proofread a later draft of the report. **Rollet** moved and **Brown** seconded to accept the report. BESAC voted and unanimously accepted the report.

PUBLIC COMMENT

None

ADJOURNMENT

The meeting was adjourned by **Hemminger** at 4:28 p.m.

WEDNESDAY, JULY 8, 2015

The BESAC meeting was convened by **Chair John Hemminger** at 8:30 a.m. EST.

PRESENTATION ON THE DIVISION OF MATERIALS SCIENCES AND ENGINEERING STRATEGIC PLANNING PROCESS

Linda Horton of BES described the Division of Materials Sciences and Engineering (DMSE) strategic planning process.

Horton reviewed the DMSE team members and individual roles. Each team has a specific focus. Division-wide themes include strongly correlated electron systems, theory and modeling and simulation, nano- and meso-scale science, advanced instrumentation, and materials synthesis. DMSE funds research that achieves a balance of grand challenge and use-inspired science.

DMSE is involved in DOE and BES strategic planning activities, as well as outreach to industry and the DOE applied offices.

BES strategic planning processes engage DMSE program managers. Reports generated from basic research needs workshops also help DMSE define its direction.

DMSE and BES support specific studies and assessments conducted by the National Academies. Published reports provide input to BES and DMSE. Horton reviewed reports that have had significant impact, to include reports on synthesis science that fed into the 2007 Grand Challenges Report and the 2015 BESAC report. DMSE funds material synthesis capabilities at the DOE laboratories and at universities. Major outputs of these studies are findings that are leveraged by external partners.

The DMSE receives input for strategic planning from the Materials Council and its workshops, National Academy studies, and interactions with DOE technology offices. DMSE Program Managers conduct annual assessments of strategic directions. The PMs identify topics for expansion and reduction, give input on hot topics, and draw on publications and other resources such as laboratory management reviews, conferences, and discussions at PI meetings to inform their input. DMSE supports strategic planning at the BES level.

Advances in the Theoretical Condensed Matter Physics Program are one area in DMSE that has evolved due to investments in research, technological innovations, and advances in planning.

The Materials Council has been around since 1969 and supports DMSE planning. It selects workshop topics and identifies emerging research needs. Council reports go into peer-reviewed journals. The Council's impact can be seen through high-impact papers and highly-cited reports.

The Biomolecular Materials Program formed in 2002 and emerged through strategic discussions going back to 1988, and several workshops and reports. Academy, Council and BESAC reports have continually defined new directions. Community input informs the emphasis for the Program.

BES and SC have been involved in strategic planning for the Materials Genome Initiative (MGI). A key piece was the DOE BES ASCR workshop held in 2010. This had a quick impact, leading to two specific activities: one on Predictive Theory and Modeling and another on Scientific Discovery through Advanced Computing (SciDAC). Funding awards for predictive theory and modeling were given in 2012. The MGI strategic plan was released in December 2014. BES co-sponsored a series of workshops looking at crosscutting challenges in the MGI area. DMSE has drawn from the MGI to guide its Materials Project. Research related to MGI includes the development of magnesium alloys with increased strength, quantum theory of exotic phases, and the ability to fill the frequency gap in solid state lasers.

The culmination of MGI strategic planning was the computational materials science FOA, which aims to deliver open source community codes and take advantage of advanced computing capabilities. Awards are expected to incorporate a strong experimental component.

Horton reviewed a timeline of BES and BESAC publications and reports, and programs and projects that have formed as a result.

Strategies are communicated on BES webpages, through presentations at professional meetings, and by video conferencing. Annual funding program announcements help convey the content of the strategic plan and guide the Early Career Award Program.

DMSE continues to support workshops and the next National Academies study. It will leverage ideas from the next BESAC report, and enhance its own communication activities.

Discussion

Barletta likes the use of workshops to drive toward the publications. He proposed an open access section at workshops to allow for broad participation through video conferencing. **Horton** liked the suggestion and offered to take it back to the Council.

Hemminger noted the focus on advanced instrumentation and asked what is funded in that arena and if it addresses the concerns in the next BESAC report. **Horton** shared that the programs support both lab and university PIs. Through mid-scale instrumentation funding in 2009, there was support for beamline activities. However, this type of activity is largely funded now through the facilities. There is still opportunity to fund smaller items with the funding cap at $2M. DMSE funds people doing work in laboratories that could be a predecessor for something larger. The program focuses on instrumentation science. Other parts of DMSE fund capabilities associated with the science around certain instrumentation. The Scattering and Instrumentation Sciences Program is funded at $64M.

Hemminger asked if there are areas within materials science that are under-represented in academia. **Horton** responded that critical areas of need are mechanical behavior and radiation effects, corrosion science, and neutron scattering.

Rollett wondered if a COV or other functions have evaluated how well funded activities are meeting strategic aims. **Horton** conveyed that COVs are asked to identify if the program portfolio is world-leading and that should in theory answer the question.

Horton shared with **de la Cruz** that electrochemistry is something that BES and DMSE looks at seriously. It is included in battery activities and corrosion research but it is underrepresented.

PRESENTATION ON THE DIVISION OF CHEMICAL SCIENCES, GEOSCIENCES AND BIOSCIENCES

Tanya Pietraβ reviewed the mission and goals of the Division of Chemical Sciences, Geosciences and Biosciences (CSGB). It embraces the discovery of grand challenge research and use-inspired basic research.

Fundamental Interactions, Photochemistry and Biochemistry, and Chemical Transformations are the three teams that make up CSGB.

The Fundamental Interactions team seeks to understand reactive chemistry at full quantum detail. The Photochemistry and Biochemistry consists of solar photochemistry, physical biosciences, and photosynthetic systems. The Chemical Transformations team seeks to characterize, control and optimize chemical change, and consists of catalysis science, heavy element chemistry, separations and analysis, and geosciences.

Beyond its core research programs, CSGB manages the Fuels from Sunlight energy innovation hub also known as the Joint Center for Artificial Photosynthesis (JCAP). JCAP started in 2010, and is led by the California Institute of Technology with LBNL as the primary partner. Research accomplishments include the discovery of a method to protect light-absorbing semiconductors from corrosion in basic aqueous solutions.

The divisional structure within BES has evolved since 2007 leading to the creation of programs within CSGB. This evolution has been informed by changing research emphases and by new research in areas to include energy capture, conversion and storage.

The Division and its three program areas are made coherent by integrative themes. Catalysis is one such area. Major questions that could solve our energy problem are how to split water, how to reduce CO2, and how to fix nitrogen. Many of these questions have been studied for decades but the answers are still incomplete.

There are core themes that are important but currently lacking in the CSGB portfolio. They include chemical synthesis, electrochemistry, self-assembly, emergent phenomena, solvation, and extreme scale computing. These areas could be given more emphasis and some are cited in BESAC reports.

The CSGB budget has stayed flat since FY09 at about $230M. The budget is allocated differently between laboratories and universities based on the discipline. In sum, 48 percent of research funding goes to universities and 52 percent to laboratories.

In FY14, CSGB gave 528 grants and 116 FWPs, and has awarded 58 Early Career grants across all programs since FY10.

Pietraβ noted that the full funding of financial assistance awards is being implemented.

CSGB's strategic planning process consists of analysis, formulation, execution and evaluation. It is guided by SC and BES, and BESAC and National Academies reports, community input, and workshops conducted by the Chemical and Biosciences Council and Earth Sciences Council.

CSGB conducts program discussions with portfolio managers to better understand their portfolios and those of their peers.

Pietraβ started strategic discussions in January 2015 with program managers to share ideas and trade knowledge. The first discussion focused on defining and assessing world scientific leadership. Subsequent discussions have addressed the budget allocation process, the visibility of CSGB research, achieving portfolio balance, and portfolio impact to ensure, among other things, that the scientific staff stays sharp and open to new ideas.

CSGB does not yet have a strategic plan from this process but has engaged in stages of analysis to answer difficult questions and enable the formulation of a plan.

Pietraβ examined news releases, DOE featured articles, and the SC website, and found that few included research that had been funded by CSGB. The SC website has several components that give information about SC-funded research and activities. Because CSGB seemed under-represented, **Pietraβ** identified ways to promote CSGB-funded research and activities through SC communication channels, and ways to disseminate results and research findings through news releases and feature articles. In the four months since executing these efforts, the number of publications, news articles and have increased versus the eight previous months.

Hiring is a concern for CSGB and the Division is striving to identify hiring needs and make strategic hires in coordination with the direction of each portfolio.

Pietraβ's goals for the Division are to support an impactful portfolio that produces highly visible world-class science in alignment with the DOE mission, and to integrate seemingly disconnected areas into a synergistic, cohesive whole.

Discussion

Cuenya pointed out that countries in Europe are aligning to work on target areas that **Pietraβ** mentioned. **Kung** noted that there are DOE-wide collaborations and laboratory-to-laboratory collaboration. With the increasing visibility of specific topics, there could be more opportunity to develop ties. Currently there are no joint funding opportunities. **Kung** confirmed for **Hemminger** that SC has not gone down this path to fund join US and EU PIs. If there are existing bilateral agreements, it would be easier to pursue. **Pietraβ** added that at the National Science Foundation, there was an international chemistry collaboration that was effective but challenging for the associated agencies due to proposal review and the investment of resources to get countries on board that might then produce proposals that were not adequate. **Horton** added that in working with the European Union, there is a big focus demonstrating the economic benefit. Once legal professionals become involved, EU ownership of intellectual property becomes part of the challenge. In terms of having PIs informally collaborate, that works very well.

Hemminger noted the discussion of areas under-represented in academia.

Hemminger felt that the issue of instrumentation and innovation seems to be missing from the portfolio. **Pietraβ** shared that instrumentation development is a component of the grants. There is no program that represents it specifically. The discussion of instrument development has not been held in the CSGB strategic discussions and **Pietraβ** is eager to hear from her program managers. **Hemminger** felt that supporting it as an integrated piece is good as the focus on the science is maintained, and that it would be interesting to know what percentage of funding goes toward instrumentation. **Pietraβ** is considering the development of a database to address those types of data needs.

McCurdy pointed out that **Horton's** earlier presentation on the BES strategic planning speaks to the strength of SC. He highlighted that the mention of coherence in materials in the BESAC report and that it might impact informational technology. That speaks to a need to remember that DOE is a mission agency. He would like to hear how the DOE mission informs decisions. **Hemminger** added that part of the mission is grand challenge fundamental science. **Kung** agreed, adding that BES takes a long view of mission with fundamental questions being part of the core of the agency.

Rollett asked about exascale computing and the status of available codes. **Pietraβ** shared that they are in discussions on the research needs and big questions that will best use the new tools.

Hemminger shared concern that the current emphases among chemistry departments does not overlap well with the needs of U.S. energy science. **Pietraβ** asked PIs if they have had difficulty attracting graduate students and that the answer was "no". At NSF, the accepted wisdom was that it is harder to attract students to physical chemistry as there is more emphasis on biological now. The question of the numbers of researchers produced and the areas in which they are produced has been debated. It must be trusted that young researchers are focused on areas of need and working with PIs who are focused on specific areas of need. CSGB must continue to support a broad base and innovation can come from unexpected corners of research.

PRESENTATION ON THE SUBTER ROUNDTABLE DISCUSSION

Don DePaolo of Lawrence Berkeley National Laboratory reported on the SubTER Roundtable Discussion held on May 22, 2015. SubTER is a working group that emerged from the National Laboratory Big Idea Summit held in March 2014. Thirteen laboratories are involved.

Subsurface engineering is critical to current and future energy systems. The main SubTER theme is adaptive control of subsurface fractures and fluid flow. Within the theme, SubTER focuses on six areas, including wellborne integrity, subsurface stress and induced seismicity, permeability manipulation, new subsurface signals, energy field observatories, and fit for purpose simulation capabilities.

By July 2015, SubTER will produce a report based on its roundtable discussion. The report will define research areas that underpin the goals of the broader SubTER Technology Team and are currently under-represented in the BES portfolio.

The grand challenge identified by the roundtable is to image subsurface stress distributions and geochemical processes. SubTER also defined three priority research directions, as well as crosscutting themes and approaches.

The problem is understanding the response of rocks to stress. The rock properties, existence of faults and fractures, and ambient stress all can influence the response. Stress can be inferred from measurements in boreholes but cannot be determined in 3D away from boreholes. It is difficult to monitor as the system is perturbed.

Fracture and fluid flow in the subsurface are a ubiquitous issue. What do the fracture patterns look like? Do they stay open?

Production of shale gas drops off considerably from year one to five. Can we got more gas coming out for a longer period of time? The number of earthquakes in the Central U.S. has gone up considerably and can be associated with high-rate injection based on a 2015 publication. There are more than 100,000 injection wells in the U.S. It is hard, however, at this time to directly associate where a well is drilled with earthquake probability.

Most of the content coming out of the wells is 95 percent water and there is no strategy for disposing of it. It is believed that seismic activity in places like Oklahoma are due to pumping the wastewater back into the Earth. When pumping water into the ground, it decreases the normal stress on faults and an earthquake is possible based on the orientation of a fault.

The biggest geothermal system in the U.S. is north of San Francisco. Water is being added to the system and producing a large number of earthquakes. Satellite data and imaging is being used to understand surface deformations.

Recent data shows that earthquakes can occur several kilometers away from where wells are being drilled. There are no firm rules on when and where an earthquake will occur based on where a well is drilled and the type of well that is drilled.

One of the priority research directions is nanoporous geomaterials and understanding their reactivity, flow and mechanics. These materials have properties that are critical for subsurface engineering issues. At times, we want to extract gas or it needs to be kept below ground depending on the purpose. The properties of nanopores and their effects on contained fluids and gases are not currently well known. The nanopores can be a large fraction of pore space.

Chemical-mechanical coupling in stressed rocks is another priority research direction. Fluid-saturated rocks can respond to induced stress in both physical and chemical ways. There are new opportunities to measure the rates of chemical reactions and response to applied stress. Models are needed to measure and monitor stress distributions.

For advanced computational methods, there is a need for a better database on material properties, chemical-mechanical coupling, and mineral-fluid reaction rates. A piece of rock can be imaged with x-rays, and then the flow and transport calculation can be determined. Permeability can vary and it is important to the outcomes over time. What happens as the fracture ages?

Architected geomaterials are an additional theme. Natural geomaterials are complicated and lab systems are too simple. Due to manufacturing processes such as 3D printing, there is the potential to make better geomaterials, more like natural ones.

The geosciences basic research needs report published in 2007 focused on carbon sequestration and nuclear waste. New issues have emerged to include fracking and geothermal energy. The short report coming from the roundtable will look at new areas that require new research for an area that is important to the energy landscape.

Discussion

Tirrell asked if subsurface emphasis focuses on shale and tight formations or if it is everything, when thinking about this effort and the focus on the water-energy nexus. **DePaolo** suggested that there is a continuum. In fluid injection, there is a need for porous material with a tight formation over to cap it. In geothermal, research is looking at hard rocks that have no permeability and hence have to be fractured. There is no emphasis on shale, but the shale business has changed the landscape. It is a rock type that has not been studied in the past.

Hemminger asked if most of the earthquakes have been deep or shallow. **DePaolo** shared that they are between a few kilometers to up to six kilometers deep.

Hemminger asked about discovery research areas described in the 2007 BES report and if geochemistry was included in the current discussion. **DePaolo** shared that geochemistry does come up in the roundtable report. However, BES asked for a description of things not being done, hence there may be less emphasis on chemistry. The roundtable looked at the connection between chemistry and physics.

Bare asked about tools and techniques, and if there are specific techniques needed for the research questions that were described. **DePaolo** shared that development is definitely needed. X-ray and neutron experiments have been breakthrough events.

Public comment

None

ADJOURNMENT

Hemminger adjourned the meeting at 11:10 a.m EST.

NEXT MEETING

The next BESAC meeting will be held February 11-12, 2016 at the Bethesda North Marriott Hotel and Conference Center, 5701 Marinelli Drive, Bethesda, MD.

The minutes of the Basic Energy Science Advisory Committee meeting held on July 7 – 8, 2015 are certified to be an accurate representation of what occurred.