Minutes
Basic Energy Sciences Advisory Committee Meeting
Hilton Washington DC/Rockville Hotel and Executive Meeting Center
Rockville, Maryland
Feb. 27-28, 2014

Members Present

Simon Bare	Max Lagally
William Barletta	William McCurdy, Jr.
Gordon Brown	Monica Olvera de la Cruz
Sylvia Ceyer	Mark Ratner
Frank DiSalvo	Beatriz Roldan Cuenya
Persis Drell	Anthony Rollett
Roger French	Gary Rubloff
Bruce Gates	Maria Santore
Sharon Hammes-Schiffer	John Spence
John Hemminger, Chair	Matthew Tirrell
John Tranquada	

Members Absent

Yet-Ming Chiang	Bruce Kay
Ernie Hall	Doug Tobias

Other Participants

Laura Biven, Senior Science and Technology Advisor, Office of the Deputy Director for Science Programs, Office of Science, USDOE
Michael Casassa, Acting Director, Materials Science and Engineering Division, Office of Basic Energy Sciences, Office of Science, USDOE
Tammy Click, Oak Ridge Institute for Science and Education
Patricia Dehmer, Acting Director, Office of Science, USDOE
Steven Dierker, Associate Laboratory Director for Photon Sciences, Brookhaven National Laboratory
Wayne Gordon, Attorney-Adviser, Office of the General Counsel, USDOE
Eric Isaacs, Director, Argonne National Laboratory
Erik Johnson, Deputy Associate Laboratory Director for Photon Sciences, Brookhaven National Laboratory
Chi-Chang Kao, Director, SLAC National Accelerator Laboratory
Carl Koval, Director, Joint Center for Artificial Photosynthesis, California Institute of Technology
Harriet Kung, BESAC Designated Federal Officer; Director, Office of Basic Energy Sciences, Office of Science, USDOE
Thomas Mason, Director, Oak Ridge National Laboratory
Robert McQueeney, Deputy Associate Laboratory Director for Neutron Sciences, Oak Ridge National Laboratory
Frederick O'Hara, BESAC Recording Secretary; Oak Ridge Institute for Science and Education
Katie Perine, Program Analyst, Office of Basic Energy Sciences, Office of Science, USDOE

Thursday, February 27, 2014
Morning Session

Before the meeting started, **Wayne Gordon** conducted the Committee's annual ethics briefing in closed session.

Chairman **John Hemminger** called the meeting to order at 9:01 a.m. Tammy Click made legal, safety, and convenience announcements. The Committee members were asked to introduce themselves. Hemminger reviewed the agenda.

Patricia Dehmer was asked to review the recent activities of the Office of Science (SC).

Lynn Orr, professor in Stanford's Department of Energy Resources Engineering, has been nominated to be the Undersecretary for Science and Energy. Marc Kastner, dean of the School of Science at Massachusetts Institute of Technology, has been nominated to be the next Director of SC. Both are awaiting congressional confirmation.

SC touches more people through its user facilities than it does through grants and employment. User facilities are an important part of SC. SC currently supports about 22,000 PhD scientists, graduate students, undergraduates, engineers, and support staff at more than 300 institutions. SC provides the world's largest collection of user facilities to nearly 28,000 users each year. There is a perception that such facilities are permanent and are never terminated. The Secretary of Energy Advisory Board (SEAB) is forming a task force on user facilities.

Of the users at the approximately 30 SC facilities, nearly three-fourths of them do their work at Office of Advanced Scientific Computing Research (ASCR) or Office of Basic Energy Sciences (BES) facilities. An additional 1700 use the Large Hadron Collider in Europe with support from the Office of High Energy Physics (HEP). For the past 30 years, each new light source has attracted new users, often from outside the field of physics (e.g., from biology). The past four Nobel prizes in medicine/biology went to SC facility users. Six years ago, the distribution of users was very different. Several of the facilities used then have closed.

A slide on facilities summarized those that were terminated and those that were brought online between 1990 and 2015. The closures include all of the big facilities of HEP, many from the Office of Nuclear Physics (NP), the "Mouse House" at Oak Ridge National Laboratory (ORNL), and many small fusion experiments. At the same time, a lot of facilities were built. So what happened to the funding of SC? In 1978, BER, BES, and computing made up about 35% of the SC budget; by 2014, that funding had increased to about 60%; high-performance computing and BES's user facilities increased significantly. HEP did not recover from the closure of the Superconducting Super Collider, and many other HEP facilities closed.

Another misperception is that SC does not know or track what is happening at the user facilities. But it does. A chart of the annual number of users shows that the total number of users at the Linac Coherent Light Source (LCLS), Advanced Photon Source (APS), Advanced Light Source (ALS), Stanford Synchrotron Radiation Lightsource (SSRL), and National Synchrotron Light Source (NSLS) increased from about 200 to over 11,000 between 1982 and 2013. This increase included a sharp rise in the number of biologists at the light sources, from about 6% in 1990 to about 44% by 2007. The National Institutes of Health (NIH) is now building and operating its own beamlines at SC facilities. BER is a large user of light sources also. The percentage of users from industry at the light sources has declined.

Statistics show that, of the users at the light sources in FY 2013, 33% are first-time users, 28% are female, 50% come from the United States, 29% come from nonsensitive foreign countries, 21% come from sensitive foreign countries, 97% conduct nonproprietary research only, 1% conduct nonproprietary and proprietary research, and 2% conduct proprietary research only. These data are used to respond to inquiries about changes or trends at the light sources.

In 2005, the technical quality of 171 operating beamlines at the four BES light sources was assessed. Each beamline was ranked in one of the categories: optimal performance (30), minor upgrade required (65), moderate upgrade required (45), major upgrade required (21), and marginally useful (10).

Under SC Director Raymond Orbach, the report, *Facilities for the Future of Science: A 20-Year Outlook*, was published in 2003. The report was a twenty year outlook and we are now at the half-way point of that projection. Funding envelopes at that time were constructed from the "Biggert Bill" authorization levels for SC for FY04 through FY08 (replaced later by H.R. 6 and S. 14), and then a 4% increase in authorization level was set for each following year until 2023. H.R. 34, the Energy and Science Research Investment Act of 2003, also known as the Biggert Bill, authorized an increase in funding for SC of about 60% from FY04 through FY07. The bill called for an increase of about 8% for FY04 followed by increases of 11%, 15%, and 15% in the following 3 years. The FY07 authorization level would have been $5.31 billion. The Office is at $4.6 billion now, so that funding envelope did not develop.

Orbach considered about 50 facility proposals, selected 30 of them, and ranked them. Here is what happened to those proposed facilities:

- The International Thermonuclear Experimental Reactor (ITER) is under way.
- The Argonne National Laboratory and Oak Ridge National Laboratory Leadership Computing Facilities (LCFs) are complete and have already been upgraded.
- The Joint Dark Energy Mission was terminated.
- The Linac Coherent Light Source has been completed and is being upgraded.
- The Protein Production and Tags was replaced with the Bioenergy Research Centers (BRCs), which are not user facilities.
- The Rare Isotope Accelerator was replaced with the less expensive Facility for Rare Isotope Beams, which is in construction.
- The Characterization and Imaging Facility was replaced with the BRCs, which are not user facilities.
- The Continuous Electron Beam Accelerator Facility upgrade is in progress.
- The ESnet upgrade is complete.
- The National Energy Research Scientific Computing Center upgrade is complete.
- The Transmission Electron Aberration-Corrected Microscope is complete.
- B Physics at the Tevatron was terminated.
- The Linear Collider was terminated.
- Analysis and Modeling of Cellular Systems was replaced with the BRCs, which are not user facilities.
- The Spallation Neutron Source (SNS) power upgrade was deferred and will be included in the second target station.
- The SNS second target station has passed CD-0, but its cost precludes a near-term start.
- Whole Proteome Analysis was replaced with the BRCs, which are not user facilities.
- Double-Beta Decay Underground Sector was funded partially; the Majorana Demonstrator is operating in South Dakota, but it is not yet the full experiment.
- The Next-Step Spherical Tokamak was terminated because of cost overruns in the National Compact Stellarator Experiment (NCSX) project; an upgrade of the National Spherical Torus Experiment was pursued instead.
- The RHIC II (Relativistic Heavy Ion Collider) luminosity upgrade was completed at a fraction of the cost and within the operating budget.
- The National Synchrotron Light Source upgrade will be commissioned in FY 2014; it is the only facility to rise in the list of priorities; the original proposal was changed at the insistence of BESAC and became one of the few new SC facilities completed.
- The Super Neutrino Beam has been partially funded; NOvA (NuMI Off-Axis Electron-neutrino Appearance Experiment) is nearly complete, but the Long-Baseline Neutrino Experiment (LBNE) is unfunded.
- The Advanced Light Source upgrade did not go forward.
- The Advanced Photon Source upgrade was funded partially; it has R&D funding.
- The Electron Relativistic Heavy Ion Collider did not go forward.
- The Fusion Energy Contingency Facility did not go forward.
- The High Flux Isotope Reactor second cold source and guide hall did not go forward.
- The Integrated Beam Experiment did not go forward.

A few facilities were started; however, after 10 years, the rank ordering was overtaken by events. The exercise needs to be redone. The Office of Management and Budget (OMB) has requested a prioritization of scientific facilities to ensure optimal benefit from federal investments. The question was put to the respective federal advisory committees [Advanced Scientific Computing Advisory Committee (ASCAC), BESAC, Biological and Environmental Research Advisory Committee (BERAC), Nuclear Sciences Advisory Committee (NSAC), and High Energy Physics Advisory Panel (HEPAP)], and OMB has been briefed. OMB's response is that the BES information was great, and they wished that all parts of SC could do as well. The BESAC report to SC made facility recommendations that were well within the funding envelope and that addressed the science, funding, etc. It was very complete and compelling.

In the FY 2014 appropriation, Congress mandated full funding for financial assistance awards of $1 million or less. As a result, SC immediately implemented this new policy.

OMB has been looking at the consolidation of science, technology, engineering, and mathematics (STEM) activities across federal agencies, putting them all within the National Science Foundation (NSF), the Department of Education, and the Smithsonian Institution. Mission agencies had a lot of STEM programs integrated into their operations. As a result, a number of DOE education programs were terminated in the FY 2014 President's Budget Request: the Computational Sciences Graduate Fellowship, Summer School in Nuclear Chemistry and Radiochemistry, Global-Change Education Program, QuarkNet for high school teachers (co-supported by NSF), National Undergraduate Fellowship Program in Plasma Physics and Fusion Energy Sciences, and plasma/fusion science educator programs. An extra $10 million from Congress will keep some of these programs going for the short-term.

The mission agencies have been asked for evidence-based descriptions of their workforce needs. BESAC will be charged to identify opportunities to meet future SC mission needs. SC plans to address these questions through expert input from independent advisors (advisory committees), program directors, and laboratory directors.

McCurdy asked about the other BESAC charge, saying that this Committee had written the grand-challenge report [Basic Energy Sciences Advisory Committee, *Directing Matter and Energy: Five Challenges for Science and the Imagination*, U.S. Department of Energy, Washington, D.C., 2007] and asking what the impact of that report had been. Dehmer said that her perspective was that the ten workshops that formed the foundation for the grand-challenge report gave a good idea of the research needed. Today, a research proposal needs to address something in the grand challenge report.

Hammes-Schiffer noted that funding for computing appeared to be flat. Dehmer said that significantly more money had been put into ASCR to serve all of SC, including BES.

Roldan Cuenya asked how much collaboration occurred outside the country. Dehmer noted that international collaboration in high energy physics is very large. The United States has the bulk of the users at the Large Hadron Collider (LHC) in Europe. The challenge is what to do beyond collider physics: elementary particles? neutrino physics? The scientific community is anxiously awaiting the report from P5 [the Particle Physics Project Prioritization Panel, a subcommittee of the DOE–NSF High Energy Physics Advisory Panel].

Rollett asked what fraction of the scientific community was involved in using these light sources. Dehmer responded that, in the 1980s, users at the light sources were dedicated to those facilities. There are now a lot of "casual" users who use the light sources for only part of what they do and who do a lot of their work back at their home laboratories. This is a huge change.

Gates asked what the dollar value of the new facilities was in comparison to the value of the facilities that were terminated. Dehmer said that the value when she started was $1.7 billion; now a huge amount of research (and facilities) has moved to the LHC, showing where science is going. This situation gives valuable insight on how science has changed with the shutdown of all high energy physics facilities. There is a story in the facilities' openings and closings on how the science is developed. The facilities are reflecting the developments in science. The whole program is dynamic.

Harriet Kung was asked to review the activities of BES.

She introduced the new hires in the Office: Ethan Merrill, Nada Dimitrijevic, and George Gardenier. Several positions in BES are vacant, including a division directorship as Eric Rohlfing has departed for another federal position. A search to fill that position is now underway. This position will shape the nature of BES's research operations and portfolio.

The FY 2014 Appropriations Conference Act was passed in mid-January. For BES, the agreement includes $24,237,000 for the fifth year of the Fuels from Sunlight Innovation Hub, $24,237,000 for the second year of the Batteries and Energy Storage Innovation Hub, $10 million (after being zeroed out by the House) for the Experimental Program to Stimulate Competitive Research, and up to $100 million for Energy Frontier Research Centers.

For scientific user facilities, the agreement provides $45 million for major items of equipment projects.

For facility operations, the agreement provides $779 million for the Synchrotron Radiation Light Sources, High-Flux Neutron Sources, and Nanoscale Science Research Centers. This is not quite the requested level of funding; it is only 97% of the optimal level of operations. This amount does include $56 million that is critically needed to start early operations of the NSLS-II at Brookhaven National Laboratory (BNL). The agreement also includes $37 million for Other Project Costs, including $10 million for the LCLS-II.

In the BES budget appropriation, Energy Innovation Hubs and Energy Frontier Research Centers are funded at FY 2013 levels, Core Research is nearly flat from FY 2013 (an increase of $6 million), and financial assistance awards of $1 million or less are fully funded for the extent of their terms. The FY 2014 appropriation of $1.712 billion rose from that of FY 2013 but was about $150 million lower than the FY 2014 President's Request.

Reductions due to the FY 2013 sequestration were absorbed by the major items of equipment (MIE) and construction funding rolloff. The increase in funding in FY 2014 raises the MIE/construction funding to approach a more normal level and enables the NSLS-II to begin early operations as planned.

The new law on full funding of financial-assistance awards means that, beginning immediately, the entire value of any grant or cooperative agreement with a total cost of $1 million or less will be obligated when the award is made instead of year by year. This is no simple matter to implement. It means all funds come out of current year funding. All available options are being used to mitigate these effects (e.g., no-cost extensions of unspent funding). The average success rate for renewals is expected to be less than 50% as compared to about 80% in the past. Overall, the success rate for the combined new and renewal applications is expected to be about 25%. While the no-cost-extension approach will afford extra flexibility to adjust for the full-funding requirement, it will also delay the time for the divisions to return to the normal portfolio size and success rates.

Another major development is the re-competition of the Energy Frontier Research Centers (EFRCs), a high-impact program. To date, these centers have produced more than 4000 peer-reviewed papers, 17 Presidential Early Career Award for Scientists and Engineers (PECASE) and 13 DOE early career awards, more than 200 U.S. and 130 foreign patent applications, and research has benefited about 60 companies. The funding opportunity announcement (FOA) for this re-competition was issued in September 2013. Nearly 300 letters of intent were received. More than 200 proposals were received. Merit review is being conducted from February through April 2014. It is anticipated that awards will be selected in May and announced in June with starting dates in September 2014. The lead institutions on the proposals are 83% universities, 15% national laboratories, and 2% industries, representing about 300 unique partner institutions from 49 states. There are about 3900 key personnel cited, of which 3200 are unique individuals. The FY 2014 Omnibus Appropriation includes $100 million for the EFRCs, compared to the annual funding level of $150 million in FY 2013 that included Recovery Act funds.

An FOA for ultrafast materials and chemical sciences was recently issued. It will provide support for hypothesis-driven research by collaborative investigative teams that combine experimental and theoretical efforts. $4 million will be available for new awards at $400,000 to $1 million per year for 3 years. Letters of intent are due by March 17; final applications are due on April 21, 2014.

The eligible jurisdictions for EPSCoR implementation grants include 26 states plus the Virgin Islands and Puerto Rico. Applications must identify a topical research area from among the DOE SC programs and/or the DOE technology offices. Support will be provided for two to three new awards at $1 million to

$2.5 million per year for 3 years. Letters of intent are due by March 22; final applications are due on April 15, 2014.

The 2014 *Basic Energy Sciences Summary Report* has been published. It provides updates to the 2011 summary report; gives an overview of BES; describes how BES does business; describes all the BES divisions, EFRCs, and Hubs; and offers representative research highlights from BES.

Recent research highlights include:

- Electrical conductivity was realized in metal organic frameworks (MOFs)
- MOFs have been shown to be a platform for new 1-D magnets
- A flexible MOF cage was devised to bind to multiple metal ions
- Biomimetic motors were devised by integrating MOFs with peptides
- Palladium atoms were isolated for highly selective catalysis of hydrogenation reactions
- A non-noble metal electrocatalyst was developed for water oxidation and oxygen reduction
- Selective catalysts were designed for the reduction of carbon dioxide to methanol
- New methods were developed for fabricating nanostructured optics that enable high-resolution, high-efficiency manipulation of hard X-rays and the exploration of new free-electron laser science
- A theoretical predicted novel electronic structure, the Hofstadter butterfly, was observed
- Light–matter interactions were controlled with meta-materials
- Dirac electrons were manipulated with ultrafast laser pulsesPreviously unobserved auto-ignition intermediates were measured

These advances are application-driven examples, and each one has a connection to a grand-challenge science.

The user numbers at the NanoScience Research Centers, in operation since 2006, continue to increase and to reach researchers from a large number of states. Most users are not from the host national laboratory; indeed, only a very small percentage of users come from the host user facility. Industry users include both large and small companies addressing disease therapeutics, ultradense memories, drug discovery, high-performance fuel cells, and advanced microprocessors. These centers have matured into fully functional highly productive research centers.

The National Nanotechnology Initiative (NNI) was launched in 2001, followed by the Hydrogen Fuel Initiative (HFI) in 2005, the EFRCs in 2009, the Solar Fuels Hub in 2010, and the Batteries Hub in 2013. All of these initiatives resulted from BESAC's charting of the portfolio roadmap. With a new charge on strategic planning for BES research, BESAC now has an opportunity to address a series of questions and issues:

- What progress has been achieved in the understanding of the five BESAC grand science challenges?
- What impact has advancement in the five grand science challenges had on addressing DOE's energy missions? With evolving energy technology and U.S. energy landscape, what fundamental new knowledge areas are needed to further advance the energy sciences? Please consider examples where filling the knowledge gaps will have direct impacts on energy sciences.
- What should the balance of funding modalities (e.g., core research, EFRCs, hubs) be for BES to fully capitalize on the emerging opportunities?
- What research areas may not be sufficiently supported or represented in the U.S. scientific community to fully address DOE's missions?

The Office is excited to work with BESAC on these issues and to take a fresh look at its research priorities and to build on the grand challenges report.

Lagally noticed the absence of "meso" topics. Kung replied that the new materials report and the NNI have meso as an integral part.

Gates stated that the new policy on full funding could have a drastic effect on science and asked what could give its implementation a softer landing. Kung responded that some grants will be funded for 2 years rather than 3; the size of portfolios has been reduced; and no-cost extensions have been used to postpone the transitions. A lot of judgments have to be made to make sure that the robustness of the portfolio is not damaged.

Spence asked if he were correct in assuming that the funding available for new programs is zero. Kung answered that it is not zero but close to it.

Hammes-Schiffer asked if the number of EFRCs would go down. Kung replied that about 33 of them will be funded.

Lagally asked if researchers should be looking for partners in EPSCoR states. Kung observed that one would have to move to those states in order to enlist those partners.

Hemminger noted that the nanoscience centers are expected to partner with facilities at the same site, but this has not worked out, in general. Kung replied that there are examples of such partnerships [e.g., between the Molecular Foundry and microscopy centers at Lawrence Berkeley National Laboratory (LBNL)]. NSLS-II will have opportunities for expanding such partnerships and synergy.

A break was declared at 10:51 a.m. The meeting was called back to order at 11:14 a.m.

Carl Koval was asked to describe the development of integrated solar-fuel generators.

The Joint Center for Artificial Photosynthesis (JCAP) resulted from the FOA for the fuels from sunlight energy innovation hub. The Center's mission is to demonstrate a scalably manufacturable solar-fuels generator using Earth-abundant elements that, with no wires, robustly produces fuel from the sun 10 times more efficiently than current crops.

The general approaches to artificial photosynthesis include: a discrete photovoltaic device wired to an electrolyzer, particle dispersions that generate solar fuels, or an integrated photo-electrochemical solar-fuel generator. No matter which approach is tried, four requirements must be met: efficiency, cost, stability, and safety. Two fuel-forming reactions can be considered: hydrogen production (water splitting) and hydrocarbon production (combining CO_2 and water). In the system, electrons have to go to an anode, and protons have to go to the cathode. However, electrons and protons move in different ways. A single photoconductor was not expected to produce the required voltage. Also, a membrane is needed that both separates the electrons and protons and at the same time conducts the protons to the cathode. An acid-stable embedded-microwire array and an alkaline-stable embedded-microwire array were developed that allow making nanodevices that split water.

The JCAP approach does not just develop materials and then put them together. JCAP designs a prototype device, figures out the processes needed for that device, and then develops the materials needed using key capabilities at various user facilities. One group develops integrated prototype devices to conduct conceptual designs of prototypes, detailed modeling of prototype design space, comprehensive design of prototypes, and fabrication and testing of prototypes. In making breakthroughs, one has to be ready to fail. A lot of prototypes are built from many designs, and a lot is learned about material integration along the way.

Recirculation of the supporting electrolyte in a water-splitting solar-fuel device eliminates large overpotentials and pH gradients. That results in a dependence of overpotential and pH on recirculation rates and allows one to evaluate a lot of designs.

Computational theory is used to model a lot of processes and designs, geometries, and types of generators. Modeling thermal effects on solar-fuel generators showed that heating up of devices cuts down on their efficiency.

Teams are made up of people with broad ranges of expertise. One idea that came out of these teams was the development of the "Q-tip design." In the fabrication process, silicon microwires would be grown via the copper-catalyzed vapor-liquid-solid–chemical-vapor-deposition (VLS–CVD) method, a metallurgical junction would be formed in the silicon, a semiconductor–semiconductor contact would be deposited on the wire surfaces by spray catalysis, tungsten oxide or titanium oxide would be deposited on the wires, and the low-band-gap material would be removed to produce a complete system.

However, the low-band-gap material does not exist, and the team has not been able to make it. So plan B was to discover inherently stable light absorbers, which was accomplished with titanium oxide coatings to protect amorphous silicon photocathodes from corrosion, allowing for efficient hydrogen production.

The real problem is the photoconductive anodes, which have experienced 40 years of failure. Production methods that have been tried include transparent conductive oxides, redox active area layers, and titanium oxide tunnel barriers. All of these techniques have failed.

JCAP tried atomic layer deposition of cobalt oxide on n-$BiVO_4$. It produces an alkaline-stable photoanode. This stabilizing catalyst film on the silicon photoanodes allowed the overpotential to remain stable for at least 24 hours. Since then, an integrated protective coating and catalyst for water oxidation has been developed. Its efficiency is equivalent to a 9.5% efficient photovoltaic in series with an electrolyzer, and its photo current is stable for more than 100 hours. It is expected that this material can produce a stable photoanode.

The JCAP Benchmarking Project serves as a community resource for the performance validation of electrocatalysts and photocatalysts. By employing a standard set of measurement protocols, unbiased evaluation by the Benchmarking Project provides comparisons that are as accurate as possible between materials/devices coming from different laboratories. Through this project, a protocol was designed, and activity and stability measurements were conducted to compare materials. More than 50 catalysts have now been processed. Only one material has been found for acidic environments, and it is not Earth abundant. The search for new materials goes on. A lot of materials have been found for a basic environment.

A high-throughput experimentation project has taken an approach of combinatorial materials synthesis, high-throughput screening, high-throughput characterization, and planning and analysis to analyze candidate materials. In addition, a fast double-screening system for catalyst activity has been developed for electrochemical characterization. Also, a scanning droplet cell that offers unprecedented speed for electrochemical measurements has been developed as a rapid-screening tool for oxygen-evolution catalysts, producing a map of current density measured at 450-mV overpotential as a function of position in a composition library. An ink-jet printed technique allowed the discovery of a high-performance cerium-rich oxygen-evolution catalyst that is stable when operating at a pH of 14. Lots of combinations were screened to see if the change in transparency produced by iron could be eliminated, and it could. Thin films of the different combinations were rapidly screened for activity.

High-throughput techniques are being used to look for efficient light architectures, tunable light absorbers, Earth-abundant hydrogen catalysts, stable and efficient photocathodes, oxygen evolution reaction catalyst mechanisms, and fundamental catalyst studies.

JCAP’s future directions include research on micro-wire water-splitting devices with greater than 10% efficiency, photocathode assemblies for combined carbon dioxide separation and reduction, plasmonic effects in electrocatalysis, and high-throughput structure determinations.

Spence asked if the new-found abundant natural gas undermines this effort. Kung noted that one of the missions of BES is to displace fossil fuels.

Rollett asked if any interesting 3-D effects had been noticed when individual cells were integrated into large systems. Koval replied that there is a group that combines components and finds unexpected results at the mesoscale.

Gates noted that Koval had assumed that devices for splitting water will aid in the reduction of CO_2. Koval answered affirmatively; CO_2 has higher kinetic barriers. The overpotential required is lower for water than for CO_2. Also, one will need a greater reactive surface for CO_2.

Lagally asked if there were a synergy between this effort and what the photovoltaic community is doing. Koval said, yes. Both communities are trying to produce voltage. However, in this program, one has to look at higher voltages because these generators need to get the highest current possible.

Ratner asked if a fundamental way had been found to get around the problem of the higher voltage needed by CO_2 reduction. Koval replied that, in another year, there will be a protocol for comparing materials for that problem. The trick will be to concentrate the CO_2 out of the air at the atomic level.

A break for lunch was declared at 12:03 p.m.

Thursday, February 27, 2014
Afternoon Session

The meeting was called back into session at 1:30 p.m.

Chi-Chang Kao was asked to review activities at the LCLS-II at SLAC. A previous BESAC report made recommended changes for the project. At BES direction, LCLS-II has been changed in response to BESAC comments.

In 2009, the LCLS saw its first light. Today, the LCLS is leading the world into a new era of X-ray science. It is experiencing rapid increases in scientific productivity and demand. At the same time, there is increasing competition worldwide. By the end of the LCL-II project, LCLS will still have a second, independent 1-km linac; three simultaneous free-electron-laser (FEL) undulator sources; operate at 120 Hz; and have a photon energy range of 250 eV to 18 keV. These changes will make new science achievable and increase the availability.

The July 2013 BESAC subcommittee recommended that the new light source have the high-energy pulse and high repetition rate necessary to carry out a broad range of coherent “pump-probe” experiments in addition to a sufficiently broad photon energy range (at least from about 0.2 keV to about 5.0 keV). The report pointed out that no proposal presented to the subcommittee met these criteria. It also recommended a robust R&D effort in accelerator and detector technology.

In response to the BESAC recommendations, the revised LCLS-II project proposes to employ the undulators in the existing LCLS tunnel with new variable gap undulators, including replacing the existing fixed-gap undulators. It also proposes to repurpose existing instruments with upgrades to access the full range of science called for in the BESAC report.

The redesigned light source will deliver high-repetition-rate science between 0.2 and 5 keV for research on catalysis, high-T_C superconductors, correlated electron systems, and *de novo* phasing with single-wavelength anomalous diffraction from sulfur. During the week following this meeting, a Single Particle Imaging Workshop was to be held at SLAC to help understand what research is needed and what milestones can be scheduled.

High-energy-per-pulse science at 5.0 to 25.0 keV will enable research on magnetic polarities of a cobalt alloy, iridate materials, phonons in superconductivity, and high magnetic fields (14 to 25 keV). This is the most efficient way to deliver a lot of X-rays in a short time. The science was the main consideration in determining the design of the machine.

This effort is a collaboration with Fermilab on cryomodules, Jefferson Laboratory on cryomodules and on the cryoplant, Lawrence Berkeley National Laboratory (LBNL) on the electron gun and its associated injector systems and on undulators, Argonne National Laboratory (ANL) on the undulator vacuum chamber and on undulator R&D, and Cornell University on R&D planning, and on prototype support on the electron-gun option. Cornell is also contributing an advanced understanding of the Q factor of the cavity to increase the energy reach.

The copper linac will produce a self-amplified spontaneous emission (SASE) beam from 1- to 25-keV proton energy with self-seeding from 4 to 12 keV. It will also produce high-repetition-rate SASE from 0.3 to 5 keV and a self-seeded grating from 0.3 to 1 keV.

The first demonstration of soft x-ray self-seeding produced a seeded bandwidth that was a factor of about 30 narrower than SASE at a photon energy of 860 eV. A seeded beam has a resolving power exceeding 5000. The 10-shot averaged spectral brightness is a factor of about 4 higher than the 2.5-mJ SASE.

Another important activity is using the existing LCLS for femtosecond X-ray diagnostics with an X-band radiofrequency transverse deflector. The electron beam is streaked horizontally and viewed on a screen in a vertically resolved energy spectrometer, revealing time-energy phase space after the FEL undulator.

The instrumentation plan is a work in progress. X-ray emission spectroscopy (XES) probes directly the electronic structures of excited states to understand the efficiency and selectivity in molecular photo-energy conversion. Each state produces a distinct signature, and XES produces a very clear view of these signatures. Resonant Inelastic X-ray Scattering (RIXS) probes charge, orbital, lattice and spin excitations. Recent research has shown the emergence of new collective modes as signatures of new states of matter, and the Q-RIXS [momentum-resolved resonant inelastic X-ray scattering] spectrometer for LCLS is ready to go. Coherent diffraction imaging using 2- to 5-keV X-rays is used to detail the RNA polymerase II complex and RNA polymerase II–mediator complex, which is a critical step in gene expression.

In laser development, nonadiabatic molecular dynamics requires ≥ 100 kHz and a < 50-fs pulse duration laser from the visible to the ultraviolet. Tracking bosonic excitations requires ≥ 100 kHz and a < 200-fs pulse duration laser. The requirements can be met by a scalable laser architecture based on optical parametric chirped pulse amplification, employing commercial kilowatt-class laser modules.

The development of detectors for imaging experiments is an ongoing program at SLAC as well as at LBNL and in Europe. SLAC tries to leverage investment and expertise within SC and beyond.

In summary, the LCLS-II design has been revised in response to BESAC recommendations; an SC-wide multi-laboratory collaboration has been formed for the project; the cost and schedule are under development; the R&D program will be focused to meet the high repetition rate science needs; and LCLS users and the wider scientific community will be engaged to exploit the extraordinary capabilities of LCLS-II.

Barletta asked how the capacity shortfall at the LCLS was going to be handled in the short run. Kao replied that a very thin crystal is used to split the beam to two instruments. One can have a larger beam, but that is harder to do.

Roldan Cuenya noted that researchers did not want to lose a minute as experiments were changed out and asked how that concern was going to be addressed. Kao responded that one spends a lot of time aligning the equipment when a change-over is made between experiments. Every experiment is different. Putting more emphasis on the engineering of the components will help. Two experiments are scheduled at once with 12 hours scheduled between the experiments.

Hemminger asked when the first experiments were expected. Kao answered that everything that can be done will be done to make it happen as soon as possible. It is not desirable for it to be too far beyond 2016.

Eric Isaacs was asked to comment on the APS upgrade at Argonne National Laboratory (ANL).

The Multi-Bend Achromat lattice (MBA lattice) will yield a 100 to 1000 times increased brightness, a huge leap for such a machine. This will create transformational opportunities in science and technology, maintaining and extending the APS's strengths for more than 5000 users with 66 simultaneous experiments, improved stability, and maintenance of the flexible bunch structure. For example, it will make possible the imaging of a single point defect, achieving the ultimate structural resolution in a bulk material.

Aggressive improvements in machine design have been made possible by advances in accelerator-modeling capabilities, the maturing of MBA lattices, improvements in magnet and vacuum technologies, innovation in the electron injection scheme, and new possibilities for high-performance undulators. The main breakthrough has been in fill-pattern flexibility: up to 4 mA/bunch.

The international consensus is that, to squeeze more power out of the beam at the right energy range, MBA lattice design for next-generation ultra-bright storage rings is the right thing to do. The upgraded APS will deliver unprecedented brightness and coherence up to high energies.

The upgrade will provide the microscope to image nanometer-scale heterogeneity and fluctuations. Transverse coherence at high energies enables imaging and spectroscopy of local structure and dynamics in real environments. Theory and simulation will be integrated. One will be able to do nanometer imaging and nanosecond dynamics via coherent scattering in challenging environments. Coherent control requires nanoscale engineering. This type of machine will serve research on cellular machinery, such as the structure and dynamics of nonperiodic systems.

The APS with the MBA lattice will vastly expand the capability and capacity of scanned X-ray probes. Resolution is now approaching 1 nm, impacting X-ray fluorescence and nanotomography, nanofocused X-ray diffraction (nanoXRD), nanoRIXS spectroscopy, and continued optics development.

At the same time, coherence enables *in operando* imaging approaching atomic resolution. APS with the MBA lattice will enable coherent diffraction imaging and ptychography with unprecedented resolution. It will also discern fast fluctuations with X-ray photon-correlation spectroscopy. This system is truly transformational, raising the question whether one can understand and create robust structural materials from the atomic scale on up for use in extreme conditions. Looking at grains can reveal stress distribution, but the upgraded APS will enable higher spatiotemporal resolution to reveal the earliest stages of deformation in complex materials.

In the microcrystallography of biological macromolecules, biologists were skeptical that new science could be enabled; but at a workshop, the advantages of the upgraded APS were seen to include the determination of 3-D structures of high-impact proteins and protein complexes. Also, the MBA lattice will significantly expand the macromolecular crystallography horizon to nano/microcrystals with an improved signal-to-noise ratio and resolution for small (0.5 to 5 μm), inhomogeneous, and/or weakly scattering crystals and reduced radiation damage. These capabilities lead one to ask whether one can unravel the molecular mechanisms of living organisms with 8000-times better 3-D resolution and higher sensitivity. It would make possible cellular imaging at about 20-nm resolution, imaging subcellular structures approaching the macromolecular scale, and whole-organism phase-contrast imaging.

With the MBA beam parameters, one can simulate coherent scattering from a single vacancy in silicon.

A grand-challenge question was, can one image and ultimately control interacting mesoscale phenomena in electrochemical systems? The APS with the MBA lattice upgrade will enable exploration of interfacial transfer dynamics, solvation dynamics, ionic and electronic mobility in solids, phase transformation and morphology evolution, and discovery of new chemistries and molecules.

One example of science being done today is the investigation of multivalent solvation structure in electrolytes, which is one way to increase battery power. The MBA lattice will enable 1000-times smaller gauge volumes containing as little as a few multivalent ions. Another example is *in operando* coherent diffraction imaging that will allow strain mapping at the nanometer scale during uptake and emission of a lithium ion in a battery. It can also be used for achieving integrated views of complex processes through time-domain ptychography as a material goes through a transformation.

This user facility will draw on the support of the research ecosystem of the national laboratory that includes transportation, protein research, nanoscience, chemical engineering, chemistry, accelerator physics, biology, materials and energy sciences, molecular engineering, and high-performance computing and data management.

The upgraded APS will exceed the other two hard X-ray machines in the world in maximum brightness across the entire photon-energy range. The upgrade will increase beam current from 100 to 200 mA and the number of bunches from 24 to 48 or 324 (depending on mode) and will decrease the horizontal emittance from 3100 to 48 or 66 pm (depending on mode).

The upgrade still needs injection systems and integration of the engineering design. There was a beam physics review in February that concluded that “the team has made outstanding progress in a short time period towards the conceptual design.” The round beam created by the MBA lattice enables great flexibility in undulators for high brightness. Research is being started on high-dynamic-range detectors and megahertz-frame-rate detectors. Computational science and data will be very important. New science will be enabled by real-time coupling of experimental data and modeling and simulation along with real-time reconstructions. A multilaboratory initiative with ASCR is being explored.

In summary, the APS upgrade with the MBA lattice will enable compelling science and technology. The design concept is well under way. The scientific community will have to be engaged. The MBA lattice is the path to the transformational understanding of matter.

McCurdy asked where time resolution was. Isaac replied that, instead of a coherent shot, many shots are taken. Once one over-samples the process, one can reconstruct the process. Generally, one is talking about working at the microsecond.

Rollett asked what the importance was of repetition rate in imaging atomic-scale defects and time-dependent behavior. Isaacs replied that, if one is getting down to a single defect, that experiment will probably take more time, but if one had the right scattering material, one can see morphologies change over time.

Spence noted that, in electrolyte solutions, the coherence is not as important as time resolution. Isaacs agreed that time rather than spatial coherence is more important.

Hemminger introduced the topic of the two new charge letters that had been received by the Committee. The first was the workforce development charge letter as input to a response to the Office of Management and Budget. BESAC is one of the expert panels that SC is reaching out to for information about gaps in workforce preparation. The response is due June 30, 2014. The Committee was to discuss the topic on this day and the following, and a subcommittee would write the report.

The other charge was on strategic planning for BES research. It is to address:

- progress on the five BESAC grand-science challenges
- the impact of that progress
- modalities of funding
- basic research areas not sufficiently supported or represented in the United States to fully address DOE's missions
- comments on workforce development

Ratner noted that another issue was big data: how does one handle it? What does one do with it? One can consider all the data, good, bad, and indifferent. Traditional views have to be supplanted with views derived from global data analysis.

Lagally did not understand the charges: Do they mean how many bodies companies need or the number of graduate students that are needed? Hemminger said that the workforce development charge is asking for input on the DOE Graduate Research Fellowship Program (GRFP). The other charge is asking the question, is the United States losing expertise in energy-important disciplines (e.g., nuclear chemistry)? Lagally asked whether internal or external needs were being talked about. Drell said that SLAC would interpret it as accelerated development of the talent needed by the LCLS upgrade. Hemminger reiterated that the charge is aimed at the GRFP, which has a broad mandate of workforce development. Are there disciplines not represented in academia where national laboratories could make a contribution?

McCurdy noted that the GRFP has been very successful. It focused on the interface of disciplines that are important to DOE. It is the best money deal DOE ever spent. The response to the charge should focus on why this educational support is needed by DOE. He was confused by the other charge: Is it an epilogue to or progress report on the grand-challenge research report, now 5 years old. The grand-challenge process needs to be revived, not just reported on.

Tirrell said that the term "disciplines" needs to be considered broadly to include instrument development.

Barletta said that there are parts of this charge that refer to the research environment that Isaacs talked about: computing, biology, instrumentation, etc. The accelerator physicists are on the ropes. One can say the same about detectors. This is a critical time. Plasma physics is needed to develop accelerators and other devices.

Rollett said that he would welcome suggestions about where to get the evidence that Dehmer had mentioned in her talk. Hemminger underscored that SC had been instructed to pull this together in an evidence-based manner. Dehmer's response was to ask the advisory committees to offer that expert advice.

Ceyer noted that the discussion had drifted away from the focus of the GRFP; the Committee needs to justify future expenditures. Dehmer wants to know what workforce development is needed to continue the efforts of the Office of Basic Energy Sciences.

Brown said that one area that needs workforce development is actinide science. NNSA put out a call for centers to train such personnel. According to a study by the National Research Council [*Assuring a Future U.S.-Based Nuclear and Radiochemistry Expertise,* Washington, DC: The National Academies Press, 2012], actinide chemistry is one of the least-represented areas of chemistry.

Roldan Cuenya said that the technical development of the user facilities is falling behind and expertise is needed to support the activities those user facilities.

Bare observed that the report should be forward looking, telling where the nation is going to go. The landscape today is very different than it was 10 years ago. The United States is now energy independent. More chemical plants have been started since fracking has increased the availability of low-cost natural gas. Core research has been underfunded for the past decade. The universities do not have the students to grow the programs. Hemminger added that that bullet is not a request for the Committee's blessing but a request for what that funding should be.

French said that, if one goes back to the grand-challenge report, some challenges have seen progress, and others have not. In the meantime, big data and analytics have come along and need to be addressed. The response to this charge needs to describe the new capabilities.

Lagally confessed to being confused by flipping back and forth between these two charges and asked the Committee to focus on one. Gates stated that it is useful to be discussing these charges intertwined. Their topics overlap. More science is becoming multidisciplinary. DOE, by offering FOAs, molds the field.

Hemminger said that the charge on workforce development will need to have a small subcommittee come up with a reply. It can identify areas whose support is justified in this program. The Computational Science Graduate Fellowship of ASCR is something that affects everyone. This Committee has to opine on and prioritize the areas that are needed. The other charge needs a workshop to consider the challenges looking forward, not backward, doing for the next 10 years what the grand-challenge report did for the past 5 years. Committee members should think overnight which of these activities they would be willing to work on.

A break was declared at 3:48 p.m. The meeting was called back into session at 4:18 p.m.

Steven Dierker was asked to present an update on the NSLS-II.

A group of new techniques will be enabled by the NSLS-II, a highly optimized X-ray synchrotron delivering extremely high brightness and flux; exceptional beam stability; and advanced instruments, optics, and detectors. It will provide best-in-class capabilities for imaging systems with nanoscale resolution and determining chemical reactivity in situ in real time. It will enable studies of interfaces and nanostructures; electronic excitations and chemical reactivity; in situ chemical, magnetic, and biological imaging; and materials synthesis, catalytic reactions, superconductors, and magnets at extremes of temperature, pressure, and magnetic field. It will produce scientific advances in clean, renewable, and affordable energy; molecular electronics; high-temperature superconductors; and structure-based drug design.

NSLS-II will have 3-GeV, 500-mA, top-off injection; a circumference of 791.5 m; and a 30-cell, double-bend achromat. It will have ultra-low emittance for high brightness and small source size. Its diffraction will be limited in vertical at 12 keV.

It will have a storage ring, linac, and booster injection system housed in a ring building, service buildings, and five laboratory/office buildings. It will be capable of housing at least 58 beamlines and will have an initial suite of seven insertion-device beamlines. Advanced optics and accelerator components will push the beam spot toward a 1-nm size.

The beneficial occupancy of the experimental floor and the commissioning of the linac and booster has been completed. Commissioning of the storage ring will start soon, early project completion is expected by August. As of the end of January 2014, the project was 94% complete, and the accelerator systems were 96% complete. The NSLS-II buildings have received Leadership in Energy and Environmental Design (LEED) gold certifications and other awards for their 30% reduction in energy use over the lifetime of the buildings.

The NSLS-II project beamlines are designed for imaging and dynamics including a coherent soft X-ray scattering beamline, a coherent hard X-ray scattering beamline, and a fast-switching polarization beamline (the only one of the world), and more. Eighteen hutch structures have been erected for the beamlines. Utility installations are 95% complete. Beamline optics installation is under way; the last optics are due in March 2014. The project is on track for an early finish.

Significant time will be required in FY 2015 and FY 2016 to install and commission the insertion devices, front ends, and beamlines. The installation schedule will be optimized and installation efforts will be coordinated with beamline operations. There will be a phased ramp-up of science capabilities, with friendly users checking out the facilities during the phasing in of commissioning.

A first-experiments workshop was held in August 2013 to update the community about NSLS-II, identify key research projects and first experiments, and facilitate the formation of teams. There were 305 registered attendees. In the first round call for proposals, 61 first light experimental proposals were received. In addition, 21 partner user proposals were received for 14 beamlines. A proposal review panel has been formed, and it met on February 4, 2014, to review all the proposals.

One first-light experiment will study electronic texture in high-Tc cuprates, which addresses a BES grand challenge. The samples are ready, the end station is commissioned, and the feasibility has been proven; the high flux of NSLS-II is needed to complete the experiment. The beamline and experiment will be science-ready by December 2014.

The Hard X-Ray Nanoprobe early-science experiments will focus on the oxidation of PtNi nanoparticles, the structures of ionic membranes, nanoelectronics, solid-oxide fuel cells, and electrochemical cells.

Dozens of workshops have engaged the community in NSLS-II. Priority research areas identified include emergent behavior from complexity, mastering materials synthesis and properties, energy systems and materials, environment and the Earth ecosystem, and structure and functions of life. Cross-cutting science themes include complexity and dynamics, functional systems, and multi-scale and mesoscale science.

Science needs drive the development of NSLS-II beamlines. An initial and near-term suite of beamlines has been set. There are eight NSLS-II project beamlines, six NSLS-II Experimental Tool (NEXT) beamlines, three ABBIX [Advanced Beamlines for Biological Investigations with X-rays] beamlines, five partner beamlines, and eight NxtGen beamlines. The ABBIX beamlines will be funded by NIH for frontier macromolecular crystallography, highly automated macromolecular crystallography, and high-brightness X-ray scattering for life sciences. The partner beamlines include Spectroscopy Soft and Tender, New York Structural Biology Center microdiffraction beamline, Beamline for Materials Measurements, and X-ray footprinting. In the next 10 years, NSLS-II will conduct world-class science with high-impact technologies. Communities are being organized in consortia to achieve greater productivity and impact. NSLS-II is working with the community to identify and develop targeted programmatic initiatives in which NSLS-II can play an active role in developing integrated research partnerships and consortia.

In summary, NSLS-II continues to make excellent progress. The commissioning is proceeding well, and early operation plans are well developed. Development of the first experiments is under way, and the user community is engaged. The team is looking forward to a fast ramp-up to an exciting science program.

Erik Johnson was asked to describe the ramp-down of the NSLS and transition to the NSLS-II.

The NSLS has had numerous science highlights and outstanding scientific productivity. It has had 57,000 users, 17,182 publications, 7122 protein databank deposits, and two Nobel prizes since 1982. It will cease operations on September 30, 2014. There has been concern about the loss of capabilities and capacity until NSLS-II is fully built out. A substantial fraction of the user community will be displaced. This displacement will be mitigated by building out the NSLS-II; identifying and communicating to users similar capabilities at ALS, APS, and SSRL; and adjusting the capacities at those alternative-host facilities.

Many of the NSLS capabilities will be turning on at the NSLS-II, but not all of those capabilities will be available right away. In 2007, a working group looked at what could be moved from NSLS to NSLS-II, identifying 14 beamlines that might realistically be moved to NSLS-II. In a 2010 call for beamline-development proposals, there was a need identified for bending-magnet, three-pole-wiggler, and infrared beamlines at NSLS-II, so the 14 beamlines identified earlier were down-selected to 8:

- Complex Material Scattering (CMS) to probe structural order in hierarchical multicomponent materials

- Quick X-ray Absorption and Scattering (QAS) for spatial and temporal study of catalytic systems in situ and in operando
- X-ray Fluorescence Microprobe (XFM; with many components scrounged from the NSLS) for characterization of chemically heterogeneous materials at the micron scale
- Tender Energy X-ray Absorption Spectroscopy (TES) for spectroscopy of multiscale heterogeneous and dynamic systems
- In situ X-ray Diffraction (IXD) for in situ and ex situ X-ray powder diffraction measurements in materials
- Materials Physics and Processing (MPP) for diffraction and scattering studies of materials
- Frontier IR Spectroscopy/Magneto, Ellipsometric and Time Resolved IR (FIS/MET) for materials science and extreme conditions communities
- Metrology and Instrumentation Development (MID), a dedicated beamline for X-ray instrumentation development

Moving these beamlines from one facility to the other is not a plug-and-play operation. The physical plants of the two facilities are quite different. Sources, front ends, and first optical enclosures at the NSLS-II will be new. Many components will need to be refurbished. As a result, the final equipment will be mix-and-match from the NSLS beamlines.

A meeting was held with BES in 2011 to assess the changes that would occur upon the transition to NSLS-II. Even with the rapid build out of NSLS-II, there will still be a reduction in capacity for several years. Of the 2,312 NSLS users in FY 2011, 507 used one, two, or three of the other DOE synchrotron facilities. However, 1805 used only the NSLS. A user transition planning forum was held in 2012 to determine how to compare light sources, and a table of different capabilities was drawn up. Existing facilities were identified that, with slight changes, could accommodate the NSLS users.

As a result, some facility modifications are under development, and there are several facilities where capability expansion has already been completed. At SLAC, the Bending Magnet Beamline 2-2 has been converted from a white beam to an X-ray absorption spectroscopy program; beam time is being provided for macromolecular crystallography at SSRL; and initial discussions are under way with other groups. At LBNL, BES has provided $500,000 to increase the IR capacity at the ALS to support NSLS users. At ANL, the APS has increased capacity at 7 beamlines to accommodate NSLS users. At BNL, the Directorate of Photon Sciences has actively coordinated with the other light-source facilities to develop specific plans to help existing users during the NSLS/NSLS-II transition. Arrangements have been made in four areas where users have been very productive at NSLS and will be strategically important to the science programs at NSLS-II. Photon Sciences will commit resources to continue to support users from these communities during the transition at other facilities, including beamline staffing, user proposal administration, and possibly loaned equipment.

NSLS staff are working with NSLS user groups to identify and develop specific plans to help them maintain their programs during the transition period by identifying suitable NSLS-II beamlines among the initial suite, working out specific arrangements with other sister facilities, and encouraging partnerships in developing and constructing specific beamlines.

The closure of NSLS will bring an end to one era and the beginning of another with the world-leading performance that NSLS-II will deliver. Thirty beamlines are under way that will provide world-class capabilities. The entire community is helping NSLS users weather the dark period at the dawn of the NSLS-II era of synchrotron radiation research.

Roldan Cuenya said that everything went well with the dedicated beamline for the Synchrotron Catalysis Consortium. It was her understanding that a beamline will not be immediately available for it at NSLS-II. Dierker replied that the program was setting up access for those researchers at other facilities and will bring up a beamline for that community in the early-science phase.

Hemminger noted that there had been a lot of discussion on the importance of integrating data management and information science into accelerator facilities and asked how that will play out at the NSLS-II. Dierker responded that the facility was developing an approach to leverage other facilities' capabilities (e.g., at BNL). Discussions are being held about setting up a central facility for data management in a two-tier manner: (1) process data in real time at each beamline and (2) send data to other facilities for storage and processing. Hemminger said that this is a huge issue. Dierker pointed out that ASCR has sponsored pilot programs at ANL and LBNL.

Lagally asked how DOE has responded to grants being lost (e.g., from NIH). Johnson responded that the NSLS has set up other facilities for them to use but have encountered such issues when such an arrangement could not be found.

Hemminger applauded NSLS's efforts to minimize the hardships during the dark period. He asked the Committee members to think overnight about involvement in the response to the two charges and in the workshop(s) involved. He opened the floor to public comment. There being none, the meeting was adjourned for the day at 5:50 p.m.

Friday, February 28, 2014

The meeting was reconvened at 9:00 a.m., and **Michael Casassa** was asked for an update of the upcoming committee of visitors (COV) to the BES Chemical Sciences, Geosciences, and Biosciences (CSGB) Division.

The very first COV in SC was the review of the Chemical Sciences portion of the CSGB Division in 2002. This is will be the fifth review for CSGB and the fourteenth COV review in BES. COVs are now a standard part of BES practice and culture and have been embraced by all offices in SC. COV recommendations are taken very seriously by BES and have resulted in substantive changes.

The current charge is of the standard format: to assess the efficacy and quality of BES processes and to comment on how the award process has affected the breadth and depth of the portfolio elements and the national and international standing of the portfolio elements.

This COV will cover base-program awards to universities and national laboratories. The base program has incorporated renewals of awards made in earlier BES solicitations and expressions of interest [HFI, Solar Energy Utilization (SEU), Nanoscale science (NSET), Chemical Imaging (CI), Single-Investigator and Small-Group Research (SISGR)]. New awards have resulted from the FY 2012 expression of interest (EOI) in Research Leading to Predictive Theory and Modeling for Materials and Chemical Sciences and from the FY 2012 Scientific Discovery Through Advanced Computing (SciDAC) FOA. These components will be of particular interest to the COV. The Portfolio Analysis and Management System (PAMS) will also be a major topic of discussion. The 2014 COV will be the last "paper" COV.

Division-wide themes include chemical imaging; ultrafast chemical sciences; nanoscale science; interfacial science; theory, modeling, and simulation; and synthesis. The Division is made up of three teams: photo- and biochemistry, chemical transformations, and fundamental interactions, with cross-cutting emphases on biomimetic catalytic systems, interfacial nanoscale chemistry, and the application of physical-science tools to biochemical systems.

Sharon Hammes-Schiffer is the chair of the COV, which will be organized into three panels, one for each team. The Chair has met with Division personnel, and conference calls will be held to review the agenda, discuss the process, and address concerns. The COV has established a website. An agenda has been developed for the COV.

Hemminger asked Casassa to say something about the recommendations from the previous COV. Casassa replied that the 2008 COV had a single recommendation: "The COV recommends, in the strongest terms, the rigorous collection of data on all aspects of proposal solicitation, review, funding recommendation, proposed action, and all metrics associated with progress that can assist in the evaluation of the impact of funded work." BES concurred, and the response has been the development of a new system for SC: PAMS. The use of PAMS started in October 2013, and that system is now being used to manage solicitations, reviews, selections, and initiation of procurement requests. It is significantly changing how BES conducts its work.

The 2011 COV had three recommendations:

- “Program Managers are encouraged to attend more national and international conferences and to make more visits to groups of researchers in their programs—to spread the message of BES programs, to encourage wider participation, and to keep abreast of forefront research in their fields.” BES concurred and has increased outreach, but travel has been increasingly restricted by appropriations. Program managers are limited to three trips per year.
- “The COV recommends continued use of the procedures applied in the program to consider short preliminary statements of research ideas (white papers) and to provide rapid evaluations either encouraging researchers to submit full research proposals or consider modifying their plans.” BES concurred, and the COV will be able to scrutinize the documents.
- “The COV recommends that BES provide web sites that are more accessible and encouraging than those currently available to those who might be interested in participating in the program and obtaining funding.” BES concurred and has a new web presence as part of the revamping of the SC website. The website’s continued evolution includes accessible information about BES programs and funding opportunities.

Hemminger noted that the report-out of the COV will occur at the summer meeting of BESAC.

Thomas Mason was asked to review the neutron science being conducted at Oak Ridge National Laboratory (ORNL).

BES investment has created two powerful neutron sources at ORNL: the High-Flux Isotope Reactor (HFIR), which has an intense steady-state neutron flux and a high-brightness cold-neutron source, and the Spallation Neutron Source (SNS), the world’s most powerful accelerator-based pulsed neutron source. Neutrons are an essential tool for addressing BESAC’s grand challenges, including understanding and controlling matter, mastering energy and information on the nanoscale, and characterizing and controlling matter very far away from equilibrium.

ORNL’s laboratory agenda is used to guide laboratory-directed research and development (LDRD) investments, strategic hires, and leveraging capabilities. Directed investments create new possibilities. In neutron scattering, a second target station at the SNS may be used for neutron imaging and the analysis of small samples. In energy-resolved inelastic scattering, a static image may be made of dynamic systems like thermo-electric materials. With the Bioenergy Science Center, biomaterials (like lignin) may be investigated to see how plants are put together, with the research results being fed into simulations at supercomputers at ORNL. In nuclear science and engineering, attention may be focused on neutron-flux effects on materials used in fusion devices. In energy systems, neutron imaging of turbine blades is supporting new energy-efficient manufacturing through such processes as additive manufacturing (3-D printing), especially on the refractory metals and specialized steels and titanium. When metals are forged, riveted, and otherwise beaten on, specific performance characteristics are produced. Currently, there is no picture of those performance characteristics for additive material components; one is needed for air-worthy manufacturing.

Robert McQueeney continued the presentation.

The vision of the Neutron Science Directorate at ORNL is derived from broad community engagement in identifying new capabilities for directing energy and matter. The near-term focus of this vision is to make better use of available neutrons, and its long-term plan is to build a second target station at the SNS.

The SNS started up in 2006; it now has 17 instruments in operation and 2 under construction. It recovered from two target failures in 2012 through enhanced quality assurance, predictable fabrication, and a new “jet flow” design. Reliability is greater than 90%. Routine operation is now at about 1.0 MW and 60 Hz, with more than 5,000 hours per year scheduled for users.

The HFIR is among the world’s highest-flux continuous sources with 12 instruments in the user program. During this past year, it was 100% predictable through six fuel cycles. It is used to produce isotopes (e.g., californium-252) and for irradiation and neutron-activation analysis of materials.

Publications from the program are increasing as new instruments come online and transition into the user program.

FY 2013 brought new instruments, new capabilities, and new communities to SNS. The IMAGINE instrument at HFIR will be used in drug design bioengineering small enzymes, pharmaceuticals, and organic compounds. VISION at the SNS will be used for chemical spectroscopy, catalysis, hydrogen-bonded solids, and optically inaccessible samples. MaNDi at the SNS will be used in drug design, bioengineering large enzymes, and membrane proteins

Extreme sample environments push neutron science to new physical regimes in magnetic fields (16 T continuous; 80 T pulsed), pressure (97 gigapascals), and in situ (hydrogen loading, stress, and batteries). In neutron-detector technology, several new areas are being pursued: helium-3 linear position-sensitive detectors, wavelength-shifting fiber detectors, and Anger cameras (used for exploring defects in lithium battery materials among other pursuits).

Software for data analysis is being moved closer to the instruments with ADARA (Accelerating Data Acquisition, Reduction, and Analysis) to improve research efficiency by managing the data flow locally, including data generation, data acquisition and control, data reduction, data analysis and modeling, comparing experimental data with simulations, and providing experiment-steering feedback.

New instruments will add science capabilities in key areas. High-throughput powder diffraction will look at small samples in complex sample environments and conduct rapid parametric studies. VENUS [Versatile Neutron Imaging Instrument at the SNS], offering wavelength-resolved neutron imaging, will be used in Bragg-edge studies and resonance absorption with less than 1-μm resolution. Cold triple-access spectroscopy will use polarized neutrons with higher resolution at higher fluxes. Other concepts are being looked at, such as neutron-spin echo and Zeemans.

A science strategy is being developed in consultation with the scientific community. Two workshops have been held: quantum materials and biosciences. Workshops covering additional topics will also be held: material synthesis and performance and soft molecular matter. Neutrons are ideal for exploring complex biological structures, where one needs to look at multiple length scales simultaneously.

A second target station at the SNS is key to meeting future science objectives that need flux, broadband, and high resolution. The second target station will ensure U.S. leadership in neutron sciences. Its short pulse provides the highest peak brightness of any current or envisioned source. Its long-wavelength beams are optimized for high brightness. And its low repetition rate provides the widest range of accessible wavelengths (length scales).

The optimization of instruments from target to sample enables groundbreaking instruments and makes performance gains by optimizing the selection of components and pulling computation into the process. The cold-neutron chopper spectrometer is expected to experience a 200-times gain, and the reflectometer is expected to experience a 100-times gain. With the second target station added to the first target station and HFIR, the complementarity among the three neutron sources would provide unrivaled capabilities. The second target station would be optimized for cold neutrons with high peak brightness. The first target station would be optimized for thermal and epithermal neutrons with high wavelength resolution. HFIR would be optimized for cold and thermal neutrons with high time-averaged brightness.

These three facilities can and will support the most potent and complete range of neutron-beam facilities available in the world, now and in the foreseeable future.

Hemminger asked what fraction of the SNS users came from ORNL, what was the percentage of subscription of instruments, and was there a big user community. McQueeney replied that the fraction of ORNL users varies by instrument. Every instrument that has been put on the floor has been instantly oversubscribed. There are no instruments that want for demand. The number of community members whose needs are being addressed has grown with the introduction of new instruments. That trend will continue. The materials community is huge. That is true for all neutron sources. About 75% of the users come from academic institutions, and the other 25% come from national laboratories and industry. There is a large component of ORNL co-authors on the publications.

Hemminger noted that local users often drive new applications of neutron sources. Mason agreed. That is happening at ORNL. They still have to go through the proposal system, though. There are people throughout ORNL that become ambassadors to their own communities. That is encouraged through the LDRD program.

Rollett asked if the ADARA data-reduction capability was developed at the facility or laboratory level. Mason replied that it was a Laboratory-level exercise. Early on, it was decided to make data management experiment-located so decisions could be made in a time-effective manner. Rollett asked what types of things could be imaged at 1 µm. Mason replied that there are trade-offs in resolution and energy. One can take the image and then do time-slicing until one gets too much noise.

Tirrell asked what was going to be done with the output of the workshops. McQueeney answered that it was hoped that they would be passed on to SC to help determine where neutron science should go. Mason added that the facility managers need to know what the second target station and the instruments need to be capable of and designed for. The desire is to field the best facility in the world. Managers also need to know what the instrument fleet should include.

Barletta asked how one balances the efforts on machine design versus instrumentation development. Mason replied that there are improvements in instrumentation that are applicable across the three facilities. The improvement of current instruments needs to be done first. The BES community is thinking about new science, and investments need to be responsive to those movements in the science. There is a time lag between the economy of the real world and that of the scientific world. The national economy is improving, and sooner or later investments in science will improve also.

Barletta asked whether enough is known from fission material modeling about the energy scaling of the damage to translate that to the fusion-reactor wall. Mason replied that, by going right into the target, one gets a lot of help; one is seeing a very compact, near-point source that all the neutrons are emanating from on the front face of the target as slowing-down neutrons in the keV range. The loops can be cooled, so one has some control over the environment. It may even be possible to load them up to produce strain. In terms of the spectrum, the fusion community has for a long time wanted to build a deuteron-driven spallation source that would produce the spectrum of interest, but that would be a major capital investment. One may be able to learn everything that is needed about radiation damage through modeling and simulation (with validation) with the hard spectrum from spallation and the somewhat softer fusion spectrum.

Laura Biven was asked to comment on DOE’s proposed response to the Office of Science and Technology Policy (OSTP) initiative to increase access to the results of federally funded scientific research.

DOE’s proposed response to the OSTP memorandum on increasing access to the results of federally funded scientific research has two aspects:

1. Data: The SC statement on digital data management is under development
2. Publications: DOE’s Public Access Gateway for Energy Sciences (PAGES) has been proposed and prototyped.

The DOE draft Public Access Plan has been submitted to OSTP.
SC’s statement on digital data management has three principles:

1. Effective data management has the potential to increase the pace of scientific discovery and promote more efficient and effective use of government funding and resources. Data management planning should be an integral part of research planning.
2. Sharing and preserving data are central to protecting the integrity of science by facilitating validation of results and to advancing science by broadening the value of research data to disciplines other than the originating one and to society at large.
3. Not all data need to be shared or preserved. The costs and benefits of doing so should be considered in data management planning.

The first requirement of the SC data management plan is that all proposals submitted to SC for research funding are required to include a data management plan (DMP) that (1) describes how data produced in the course of the proposed research will be shared and preserved or (2) explains why data sharing and/or preservation are not possible or scientifically appropriate. At a minimum, DMPs must describe how data sharing and preservation will enable the validation of results or how results could be validated if data are not shared or preserved. DMPs will be reviewed as part of the overall SC research proposal merit review process. The DMP guidance will have caveats on the treatment of national security data and the like.

The second requirement is that DMPs must provide a plan for making all research data displayed in publications resulting from the proposed research digitally accessible at the time of publication. This includes data that are displayed in charts, figures, images, etc. This requirement could be met by including the data as supplementary information to the published article or through other means. The published article should indicate how these data can be accessed.

The third requirement is that researchers who plan to work at an SC user facility as part of the proposed research should consult the published data policy of that facility and reference it in the DMP. The facilities are to put their DMPs on their websites.

The term “digital data” encompasses a wide variety of information stored in digital form, including experimental, observational, and simulation data; codes, software and algorithms; text; numeric information; images; video; audio; and associated metadata. It also encompasses information in a variety of different forms, including raw, processed, analyzed, published, and archived data. Software is included in this definition.

The requirements will apply to all proposals for research funding regardless of institution but not to applications for time on user facilities. At some point in the future, requirements will apply to proposals submitted in response to all SC research solicitations and to invitations for new, renewal, and some supplemental funding.

On the publication side, the results of unclassified research that are published in peer-reviewed publications directly arising from federal funding should be stored for long-term preservation and publicly accessible to search, retrieve, and analyze. Public access to the best-available version of a scholarly article is to be assured within 12 months of its publication. The “best-available version” might be (1) the version of record published and hosted online by the publisher or (2) the accepted manuscript hosted online by the publisher, a third-party repository (e.g., Lab, arXiv, or an institutional repository), or the DOE Office of Scientific and Technical Information (OSTI).

For the last option, OSTI would use a proposed tool, PAGES, to obtain metadata about DOE-funded publications and to provide links to the online versions of those original publications. As designed, PAGES allows keyword (including author name) searches to retrieve abstracts, metadata, and links to full articles (the version of record) when available. A prototype of PAGES has been developed.

Another of the access options, publisher online hosting, may be achieved through CHORUS, the Clearing House for Open Research of the U.S. About 90 publishers are signatories to CHORUS, potentially covering about 90% of DOE peer-reviewed publications. CHORUS is currently evolving; seven publishers are active in a CHORUS pilot project that contains about 4000 journal records. All publications in CHORUS will be available through PAGES. Participating publishers agree to make articles resulting from federal funds publically available “after the determined embargo for each discipline and agency.” The CHORUS project provides freely consumable metadata for these articles, including seamless links to the publisher’s version of record for tools like PAGES. Articles resulting from federal funding are to be identified by additional metadata fields with FundRef support from the publishers. OSTI is a member of FundRef.

Hemminger commented that in interactions with publishers some of them are very aggressive.

Gates asked what the implications were for profit-making publishers. Biven replied that no one knows yet.

Bare asked for clarification on the situation where a researcher does not get federal funding. Biven replied that, in that case, one does not need a DMP.

Hemminger asked if any facilities had announced what their data management plans were going to be. Biven replied that many facilities already have DMPs in place.

Roldan Cuenya asked if there were any standards about database use. Biven answered that guidance would be provided to DOE’s researchers.

Gates noted that one can produce unlimited data that has little meaning to the uninitiated. The implications of making it useful would require a lot of effort to make it understandable. Biven responded that one has to determine what data require curation. Then one can rely on the research community to interpret it.

Lagally noted that what data needs to be curated seems to be narrowing down in this discussion and asked for more details. Biven replied that each project office is developing guidelines. Rubloff asked if there were a provision for author identification so individuals can be distinguished. Biven agreed that that would be good. Rubloff asked if the sharing of illustrations were allowed. Biven answered that that would be up to one's facility's DMP.

Roldan Cuenya asked whether the extra work that will be required will be covered by grants. Biven said that that is the plan.

Bare asked why results are being made available to competitors. Biven replied that there is no metric yet, but there will be.

Hemminger said that he had received input on the charge subcommittee overnight. For the longer charge, there is enthusiasm for participation in a workshop on what the future looks like. He will seek volunteers to work on that workshop, which would have several components.

The other charge can be dealt with quickly. The desire is to identify disciplines that are not well represented in academic curricula, to identify DOE-mission-relevant disciplines that are in high national or international demand, to identify high-demand disciplines for which the national laboratories can provide workforce development, and graduate and postdoc courses that could address workforce-development needs. Disciplines that people have mentioned as being in need are computational science, accelerator science, detector physics, actinide science (nuclear and radiochemistry), fundamental electrochemistry, crystal growth, mechanical properties of water at the nano and meso scales, and neutron scattering.

McCurdy said that the term computer science is too broad and needs to be broken down. That is what the Computational Science Graduate Fellowship of ASCR used to address. The other disciplines cited seemed narrow. Ultrafast science is not there; BES just had an FOA in that area, and the LCLS-II will operate largely in that area. He suggested a broader list that was more oriented toward energy.

Hemminger said that he expected that a letter report would be produced and that the introduction should say many of those things. He will need some help writing it. It will not be long.

DiSalvo stated that crystal growth is a broad area. It is not just someone to make stuff for researchers. It involves many methods that need development. It involves computational approaches.

Brown said that, in chemistry, actinide science is the least-supported area. It is almost unique to DOE's needs. It is narrow, but essential to DOE's mission.

Hemminger noted that accelerator science and detector physics have been flagged as critical to the development of DOE facilities. Actinide chemistry is another such area. Computational sciences is broadly practiced and used. It is not specific to DOE missions, however, but is essential.

Spence said that there should be a focus on instrumentation and areas in which the United States is falling behind. Universities need courses in, say, XFEL [X-ray free-electron laser] science.

Bare said that one also needs to think along the line of beamline scientists to accommodate enhancement of current instrumentation as well as new instruments. The expanded use of the facilities may make up a paragraph in the report.

Hemminger asked whether there were any graduate research fellows in ASCR working on data management. McCurdy said, yes. That fits the last bullet very well. The ASCR Computational Science Graduate Fellowship requires at least a summer internship at a national laboratory and an extended presentation of the fellow's results.

Rubloff wanted to see electrochemistry broadened significantly.

Barletta said that accelerator science and detector physics apply to current facilities and instruments as well as to future facilities. There has to be a tie-in between the students and the DOE facilities. Students do things at the facilities that are not available on campuses.

Hall said that there are broad impacts on BES of computational science (e.g., the data) that are not well represented in academic curricula.

Ratner said that students need information that is not provided in classes; plus, as students go to summer programs, they get to know each other and build networks for information exchange.

Brown stated that there are a lot of broad energy areas that are needed (e.g., environmental damage).

Olvera de la Cruz noted that, in software development, there is a lot of work to be done.

Tranquada said that neutron scattering is on the list because 14 years ago, no PhD candidates with experience in instrumentation could be found. The only way students can learn about instruments is at the facilities where those instruments are. It is part of the instrumentation problem along with data management. It needs people who know what data are needed and how to analyze and characterize the data.

Gates said that the Committee should think about mentors and about distinguishing between postdocs and graduate students (who need to be matched with appropriate mentors). Hemminger said that one of his students went to the ALS and suddenly had a number of mentors, not just one.

Roldan Cuenya pointed out that mentors at a university might have a narrow experience with a given instrument, but training programs at facilities could introduce students to a variety of instruments.

Barletta described a 2-week short course at Fermilab about 5 years ago in which a mentor was assigned to each student to guide the student through a summer research project that would become their senior thesis.

Drell said that this is orthogonal to anything NSF would do, which is good. It also needs to be orthogonal to the grants normally available for postdoctoral programs and fellowships.

Hemminger asked for volunteers to help write and edit the report. About seven members responded. Kung assembled a roll of the volunteers. A draft of the report will be produced and circulated to the Committee members.

For the other charge, a schedule for the workshop(s) and what it (they) will look like will be drawn up.

McCurdy said that the Committee has to lay out a roadmap for energy research in the changing landscape, as affected by petroleum and natural gas production. Brown added that a roadmap was also needed for facilities and what capabilities they need. Ratner pointed out that, in dealing with fracking, one needs to deal with politics. The scientific community needs to help people who produce public policies. That is important. Hemminger said that it is important but the Committee knows nothing about policy formation. Olvera de la Cruz said that she participates in a discussion of briefing the private sector on the science behind policymaking. DiSalvo said that the administration has said that natural gas should be used to build a bridge to a low-carbon future. The Secretary is concerned that the natural gas would be used up but that the bridge would not be built.

Gates said that one needs to figure out how energy is linked to the environment. Hemminger pointed out that this is a BES advisory committee; the Office of Biological and Environmental Research (BER) covers environmental research. It would be dangerous for this Committee to get into BER’s territory. What is needed is to figure out what BER is not doing.

Barletta noted that almost all the current nuclear plants will be gone in 50 years. The aging of materials requires accelerated testing and research. This is critical to the energy future of the United States.

Hemminger invited Committee member participation in the workshop and called for additional comments.

Rollett asked if there were any time frame for the workshops. Hemminger replied that the earliest that a workshop could be held would be in the summer, but there is a lot of discussion that needs to be done beforehand. It should not be rushed. It is an information-gathering exercise and will produce a report like the one prepared for the grand-challenges charge.

Bare said that the workshop should not focus on the first bullet. That first bullet could be done now. Hemminger agreed that the first bullet could be done by the writing group.

The next meeting of the Committee was set to be July 29–30, 2014, at the Marriott Bethesda North Hotel and Conference Center.

The floor was opened for public comment; there being none, the meeting was adjourned at 11:39 a.m.

Respectfully submitted,
Frederick M. O’Hara, Jr.
Recording Secretary
March 24, 2014