Minutes
of the
Basic Energy Sciences Advisory Committee Meeting
August 5–6, 2010
Hilton Rockville Hotel and Executive Meeting Center
Rockville, Maryland

BESAC members present:

Simon Bare
Sylvia Ceyer
Sue Clarke
Peter Cummings
George Flynn
Bruce Gates
Laura Greene
Sharon Hammes-Schiffer
John Hemminger, Chairman
Bruce Kay
Kate Kirby
William McCurdy, Jr.
Martin Moskovits
John Richards
Douglas Tobias
John Tranquada

BESAC members absent:

Nora Berrah
Frank DiSalvo
Mostafa El-Sayed
Daniel Morse
John Spence
Kathleen Taylor

Also participating:

Paul Alivisatos, Deputy Director, Lawrence Berkeley National Laboratory
Harry Atwater, Division of Engineering and Applied Science, California Institute of Technology
William Barletta, Department of Physics, Massachusetts Institute of Technology and University of California at Los Angeles
William Brinkman, Director, Office of Science, USDOE
Patricia Dehmer, Deputy Director for Science Programs, Office of Science, USDOE
Gregory Exarhos, Associate Director, Fundamental Science Directorate, Pacific Northwest National Laboratory
Roger French, Research Fellow in Materials Science and Engineering, Central Research and Development, DuPont Co.
Linda Horton, Director, Materials Science and Engineering Division, Office of Basic Energy Sciences, USDOE
Janos Kirz, Department of Physics and Astronomy, Stony Brook University
Steven Koonin, Under Secretary for Science, USDOE
Harriet Kung, Associate Director of Science for Basic Energy Sciences, USDOE; BESAC Designated Federal Officer
Nathan Lewis, Division of Chemistry and Chemical Engineering, California Institute of Technology
Alex Malozemoff, Chief Technical Officer, American Superconductor Corporation
David Miller, Director, Science and Engineering Division, Idaho National Laboratory
Pedro Montano, Director, Scientific User Facilities Division, Office of Basic Energy Sciences, USDOE
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Katie Perine, BESAC Committee Manager, Office of Basic Energy Sciences, USDOE
Geraldine Richmond, Department of Chemistry, University of Oregon
Eric Rohlfing, Director, Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, USDOE

John Sarrao, Science, Technology, and Engineering Directorate, Los Alamos National Laboratory
Leslie Shapard, Oak Ridge Institute for Science and Education
Marvin Singer, Senior Advisor, Office of Basic Energy Sciences
Dion Vlachos, Department of Chemical Engineering, University of Delaware

About 110 others were in attendance in the course of the two-day meeting.

Thursday, August 5, 2010
Morning Session

The meeting was called to order by Chairman **John Hemminger** at 8:39 a.m. **Leslie Shapard** made safety and convenience announcements. Dr. Hemminger asked the members introduce themselves and then reviewed the agenda.

William Brinkman[1] was asked to give an overview of activities in the DOE Office of Science (SC). Dr. Brinkman noted that President Obama is supportive of science. He quoted the President as saying, "When we fail to invest in research, we fail to invest in the future." Dr. Brinkman reviewed the structure of the Office of Science and its budget. SC has six research offices and the Office of Workforce Development for Teachers and Scientists. SC's priorities include scientific computing and climate science. The SC budget request for FY11 is $5.1 billion, a 6.1% increase.

The 2011 budget has now come out of the congressional committees. SC took a heavy hit in the House markup (nearly $240 million before earmarks). And the Senate took $150 million away from the request (again, before earmarks). There were $18.3 million in unfunded directed earmarks added in the House markup and $40.8 million added in the Senate markup.

The SC Graduate Fellowship Program is very important. In FY 2011, $10 million will be available to fund about 170 additional fellows. About $16 million will be available in FY 2011 to fund about 60 additional Early Career Research Program awards at universities and DOE national laboratories.

The ultimate goal for the Fuels from Sunlight Hub is to imitate photosynthesis with a factor-of-10 increase in productivity. The winning team was California Institute of Technology and Lawrence Berkeley National Laboratory (LBNL). It will be led by Nate Lewis and will partner with six other institutions. The Department is pushing for a Battery and Energy Storage Hub that will deal with the problems produced by intermittent energy sources (wind, solar, etc.). It is in the Senate version of the FY11 budget.

The Office of Advanced Scientific Computing Research (ASCR) has an Exascale Initiative. The major components of the Exascale Initiative include

- Platform R&D;
- Critical technologies;
- Software and environments;
- Co-design; and
- Early prototype platforms.

[1] Dr. Brinkman's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

The Linac Coherent Light Source (LCLS) at SLAC produces an amplified X-ray beam and has already produced several science results, such as refracting nanocrystals in water.

The International Thermonuclear Experimental Reactor (ITER) project in the past year has developed a real schedule, estimated a realistic cost, and installed a new director. It has been established as an independent international legal entity with about 400 personnel from all of the member nations. The United States has a 9% share in this enterprise. Roughly 80% of the U.S. contribution will be in-kind components manufactured largely by U.S. industry. In addition, the United States will contribute 13% of the cost for operation, deactivation, and decommissioning. The U.S. share of construction was estimated to be $1.45 billion to $2.2 billion. ITER is located in Cadarache, France, and the site has been prepared.

In particle physics, SC is supporting work at the Large Hadron Collider (LHC) and at the Long-Baseline Neutrino Experiment. There is a big push to keep the Tevatron running. The LHC is slow in starting up. It is not clear how the ramp-up of the LHC is going to proceed. The Tevatron was to have been shut down in 2011, but areas of exclusion for the Higgs boson have been constantly expanded, leading to valuable prospective insights from its continued operation for another 2 or 3 years. But extending the operation of the Tevatron will be expensive. An advisory committee will consider the question of its continued operation later this summer.

Steps are being taken to strengthen the Small Business Innovative Research (SBIR) program, which amounts to $150 million to $200 million per year in the DOE budget. Those steps include moving the office to report directly to the Deputy Director of SC.

Dr. Brinkman answered questions posed by the panel.

Question: There has been a long history of a Graduate Research Fellowship Program in ASCR. What will happen to that program?
Answer: ASCR's fellowship program will not be affected. Congress did not give DOE money to expand the program next year. The Graduate Fellowship Program should have been pushed more strongly.

Question: Will funds for the accelerator-science fellowships and internships be affected?
Answer: Dr. Brinkman said that he would like to see more summer jobs at the national laboratories.

Question: What is the status was of the other three hubs.
Dr. Brinkman responded that the original three hubs are pretty much on the way. He is hoping to do one more this fall.

Comment: There seems to be a general impression that Congress is confused about the potential overlap of programs. For example: the EFRCs vs. the Advanced Research Projects Agency–Energy (ARPA-E).
Answer: Dr. Brinkman said that such confusion is a problem. A way has to be found to make the case more clearly.

BES Director, **Harriet Kung**[2] was asked to review the activities of BES.

[2] Dr. Kung's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

BES has joined with ASCR to sponsor a workshop on Computational Materials Science and Chemistry for Innovation. The report, *Science for Energy Technology,* is out. It has the results from nine panels and presents 29 priority research directions (PRDs). It will be described later in this meeting. The report discusses two kinds of science contributions:

- breakthroughs that change the technical landscape; and
- understanding and ultimately controlling existing phenomena, underpinning technological revolutions.

This report is focused on producing a near-term industry impact.

The Workshop on Accelerator Physics of Future Light Sources had as its main goal to evaluate the state of readiness of machine architectures to building the next major X-ray science user facility. From this workshop, five reports will be published in *Nuclear Instruments and Methods in Physics Research, Section A.*

The Compact Light Sources Workshop looked at alternatives to major synchrotron facilities. It considered inverse Compton sources, high-harmonic generation, plasma sources, plasma-based accelerator sources, and compact storage rings. BES will now have a good understanding of the current state of the art and future research needs as it plans for the next generation of light sources.

Forty-six EFRCs have been launched, and 16 more would be supported by the FY11 budget request. They are designed to engage the nation's best researchers to address research gaps. Each of the 46 centers has undergone reverse-site peer review, the first step in the management and operational review of the centers. All 46 centers were reviewed in 3 months. The purpose of the reviews was to help each center get the best start possible by identifying best practices and identifying and addressing any operational issues that may impede progress. The results of the reviews were furnished to the center directors. A compilation of good practices for each of the centers will be assembled and distributed as a resource.

The Fuels from Sunlight Energy Innovation Hub is the Secretary's signature initiative. The objective of the hub is to develop an effective solar-energy-to-chemical-fuel conversion system that would operate at an overall efficiency and produce fuel of sufficient energy content to enable transition from bench-top discovery to proof-of-concept prototyping. Highly integrated research teams at a hub allow advances an individual researcher cannot achieve. The award for this hub was announced on July 22, 2010, to a team led by Nate Lewis, of Caltech, and LBNL. The award has a startup date in September 2010. Its R&D will focus on the robustness of components and the acceleration of the rate of catalyst discovery for solar-fuel reactions.

BES has been completing the LCLS construction project, with CD-4 [Critical Decision 4] being granted in June 2010, one month ahead of schedule. Each component was completed on time, meeting or exceeding all technical specifications. The first experiments were conducted in October 2009. In one experiment, a neon atom was stripped bare of all ten electrons from the inside out via inner-shell photoionization, producing "hollow atoms." The data produced reveal mechanisms of radiation damage. Another experiment studied X-ray-induced ionization, dissociation, and frustrated absorption in molecular nitrogen.

Another construction project is the National Synchrotron Light Source upgrade (NSLS-II). Groundbreaking was held in June 2009, and the storage ring is almost completed in August 2010. This construction project was aided by $150 million of ARRA funding. More beamlines need to be added to the NSLS-II. NSLS-II EXperimental Tools (NEXT) will add five or six beamlines, increasing user capacity by 300 to 400 users. CD-0 for this expansion was approved on May 22, 2010.

The Advanced Photon Source is undergoing an upgrade. It has 3,500 users annually and is one of only three such facilities in the world. The others have already been upgraded. Key components will include accelerator and X-ray source upgrades, new and upgraded beamlines, and new technical capabilities. The goal is to provide an upgraded third-generation synchrotron light source facility that provides an unprecedented combination of high-energy, high-average-brilliance, and short-pulse X-rays together with state-of-the-art X-ray beamline instrumentation to reveal the microstructures of systems investigated. CD-0 for this upgrade was approved on April 22, 2010.

An expansion of the LCLS (LCLS-II) is being proposed to extend the spectral range and control of X-ray polarization for the study of charge and spin order, to increase control of pulse intensity and length, to produce temporally coherent beams with reduced bandwidth and increased peak brightness, and to allow simultaneous operation of experimental stations to accommodate the fast-growing number of users. This expansion will present a cost-effective and timely plan for U.S. fourth-generation light sources. CD-0 was approved on April 22, 2010, and marks the start of the conceptual design phase.

Appropriations will be needed for these projects to go forward. The upgrades of the light sources allow more users, and BES takes its stewardship role very seriously as it looks to the needs of the scientific community during the next 10 years.

The BES FY11 budget request is for $1.835 billion. The FY11 request would increase funding for the energy innovation hubs, the EFRCs ($40 million to cover under-represented topical areas in carbon capture and advanced nuclear energy systems and in discovery and development of new materials), and core research for grand-challenge science, use-inspired science, and accelerator and detector research.

On the facilities side, the NSLS-II construction will continue and optimal operations of the scientific user facilities will be funded. The Senate Energy and Water Development appropriations markup recommended funds for construction activities and for the current 46 EFRCs. No funding for additional centers was recommended. Full funding for the Fuels from Sunlight and Batteries and Energy Storage hubs was recommended. Gas-hydrates research was referred to the Office of Fossil Energy, not SC. The Experimental Program to Stimulate Competitive Research (EPSCoR) was funded at $35 million. No funding was recommended for modeling engine design ($20 million had been requested). The Senate markup was $95.9 million below the request and $102.6 million above the FY10 appropriation.

Unofficially, the House markup is $150 million below the request with no additional funding for EFRCs or for the proposed Batteries and Energy Storage Energy Innovation Hub. Both markups provide full funding for construction activities and allow for near-optimal operations of science user facilities. They differ on EPSCoR and hubs and leave reduced or no funds for new research activities. This is a major setback for BES and a loss of several research opportunities. Both markups keep BES off the budget-doubling track. However, BES has made great strides forward in investments in scientific areas in the past few years.

New staff have been added in BES Operations, Materials Sciences and Engineering Division leadership, and the Facilities Upgrade Program. Program managers will be joining BES in Fuels for Sunlight and EFRC oversight. There are vacancies in Condensed Matter Physics, the coordination of the EFRCs, and User Facilities.

Dr. Kung thanked the paned for its guidance and support. She then answered questions posed by the panel.

Question: What areas are not covered by the EFRCs?
Answer: Carbon capture, radiation resistant materials, actinide science, and materials and chemistry by design.

Question: What about a crystal-growth center?
Answer: There is no flexibility for that in the House mark. Perhaps the Senate mark will allow it.

Question: How many proposals had been submitted for Fuels for Sunlight.
Answer: There were several, but the number could not be revealed now.

Question: What is the timeframe for the upgrade of the Advanced Photon Source (APS)?
Answer: It is too early in the design phase to be able to set a timeframe for the upgrade.

Question: Why was it possible to go fast for the NSLS-II ring and what has been learned from the experience?
Answer: Funding up front allowed the acceleration of construction. Uncertainties and risks (such as future costs of materials and labor) were brought down. In addition, market conditions allowed a good deal on construction costs.

Question: What efforts were being made to ramp up the user base at the Spallation Neutron Source (SNS)?
Answer: Slow commissioning and slow installation of instruments has hampered recruitment of experimenters, causing the ramping up of users to be sluggish. Several recommendations have been sent to the SNS.

Question: What can you say about the funding, capabilities, and users of the Nanoscience Research Centers?
Answer: All five centers are up and running, and some are saturated in users. Funding is sufficient to allow optimal operation of the centers. Capital equipment costs are now being covered. A review of all the centers is being completed, and they all seem to be doing well.

A break was declared at 10:16 a.m. The meeting was called back into session at 10:32 a.m. to hear **Geraldine Richmond**[3] report on the Committee of Visitors (COV) to the WDTS.

When this COV was charged, the FY10 budget request for WDTS was $20.7 million, more than double the FY08 appropriation of $8.0 million and nearly double the regular FY09 appropriation of $13.6 million. WDTS also received $12.5 million of ARRA funds in FY09 to begin a new SC Graduate Fellowship Program. It has a lot of visibility. The COV was asked to review the quality of programming of student programs, educator programs, and a broad category of other small efforts. It was charged to assess the efficacy and quality of the processes used to solicit, review, recommend, monitor, and document application, proposal, and award actions; to evaluate

[3] Dr. Richmond's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

the plans for the new graduate fellowship program; and to examine current and future staffing needs for the WDTS program.

The overall findings were that the Division operates with many dedicated staff and a Director who are fully committed to its success. It contains several programs that play a unique and important role in U.S. science workforce development. Several programs of the highest quality do not have sufficient resources to allow them to reach their full potential. Assessment of the quality and impact of all programs is completely inadequate. Procedures and policies for establishing new programs are absent. And there is little or no connection between the DOE staff in Germantown and scientists, staff, and research activities.

The Science Undergraduate Laboratory Internship (SULI) is a flagship DOE program that provides internships to undergraduates at national laboratories. It is rated as excellent but can be improved. It is poorly advertised and not diverse. Inadequate assessment and evaluation make it impossible to understand how it compares with similar programs like the Research Experiences for Undergraduates (REU) of the National Science Foundation (NSF).

The Community College Institute (CCI) is rated as good with potential for excellence. It is a small but promising program (49 students in 2009) designed to attract community colleges' diverse population into science and engineering. It has a diverse body of students, many of them first-generation college students. It needs to expand but also to improve on evaluation and assessment.

The SC Graduate Fellows Program is rated as very good with the potential for excellence. The program staff and awards should be expanded.

The National Science Bowl (NSB) is rated as excellent. This is the original National Science Bowl in the United States. Its weaknesses are that the final event at the National 4H Center is approaching saturation and that the regional competitions' geographic coverage is arbitrary. This program should be expanded to underrepresented areas of the country, and regional science bowls should be conducted to lead up to a final contest in D.C.

The Real World Design Challenge is rated as poor. This is a small engineering and computer-aided-design program to develop low-drag aircraft wings. This program should be terminated, and the resources shifted to stronger programs.

The Pre-Service Teachers program is rated as poor. It should be terminated, and the resources shifted to stronger programs.

The Einstein Fellows program is rated as very good. It is a high-quality experience for high school and community college teachers. Its goals are not always clear. It has the potential for underutilization of talent if participants become merely "filler." The articulation of the goals of the program should be improved and uniformity should be imposed on tasks.

Faculty and Student Teams (FaST) is rated as fair. There was not enough quality in the program. It has become localized around the national laboratories rather than a national program. Follow-up is not good. It should be terminated, and the resources shifted to stronger programs.

Academies Creating Teacher Scientists (ACTS) is rated as good to fair. In it, teachers are introduced into research activities at the national laboratories. It could be sponsored locally by national laboratories. This program should be terminated, and the resources shifted to stronger programs.

The Lindau Awards take graduate students to meet Nobel laureates. It is rated as excellent. There are excellent connections with the program officers at Germantown. It should be used as a model for other program operations.

The Equipment Donation Program provides equipment to high schools, community colleges, and universities. It is rated as good. However, there is no significant follow-up to make sure equipment has been put to use and maintained. If this program is continued, modifications are necessary.

The College Planning Guide was started a number of years ago to instruct students how to apply to college. It is redundant with other efforts. It is rated as poor. This program should be terminated, and the resources shifted to stronger programs.

The Science and Energy Research Challenge (SERCh) poster competition is rated as poor. It would be better to send students to a national laboratory scientific meeting. This program should be terminated, and the resources shifted to stronger programs.

The *Journal of Undergraduate Research* publishes papers from students from DOE national laboratories. It is rated from fair to poor. There are other peer-reviewed journals that these authors can publish in. This program should be terminated, and the resources shifted to stronger programs.

Dr. Richmond answered questions posed by the panel.

Question: How were the evaluations were carried out?
Answer: The COV met with the Director, had a conference as a group, and split into three groups. Program managers briefed each group (except one) on their areas of expertise. The self-assessment level was low. The COV had a plenary session to talk to program managers. It then produced a consensus report. Its overall recommendations were for WDTS to focus its efforts and resources on its strong programs and to work to improve and expand them to assure future success and impact. It should redirect funds from the weak programs. It should add PhD-level scientists to the staff who have experience in scientific research, educational outreach, and grants. The management team should work in to increase the participation of students and scholars from underrepresented groups. The level of interaction, cooperation, and coordination between staff in WDTS with SC programs and program officers should be increased. The procedures used in the solicitation and selection of the graduate fellows should be improved, building on the experience learned in the first year. Assessment and evaluation procedures should be developed and implemented for the programs that meet the standards of similar programs in other agencies, such as NSF. These assessments should be used on a regular basis to improve and modify existing programs. The procedure that is routinely used in SC in developing new programs should be followed. There should be buy-in from the affected communities.

Question: What kind of funding levels were to be shifted?
Answer: They are not very large, perhaps a total of a few hundred thousand dollars.

Comment: The report should be given to all the national laboratories. Also, the undergraduate research journal could be made a web-based archive of undergraduate research.

Answer: The COV struggled with the undergraduate research journal a lot but felt it was redundant and noted that the papers were selected by an office that had no science PhDs. It needs a peer review, and there is not a staff for that.

Comment: Tracking of participants would allow supporting such programs before Congress.
Answer: There is not any such tracking. It is difficult to do and requires a lot of manpower. However, it does need to be done.

Question: How much do people associate DOE with these programs?
Answer: That is a good question. The link is largely missing.

Chairman Hemminger asked for a show of hands for acceptance of the COV report. The vote was unanimously positive.

Nathan (Nate) Lewis[4] was introduced to give a seminal view of the Joint Center for Artificial Photosynthesis (JCAP). The Secretary issued a bold challenge that deserved a bold response. The JCAP has a startup-company approach with a highly focused research agenda. It has two divisions: Accelerated Discovery and Science-Based Scale Up. It has eight partners in the form of two national laboratories and six research universities. It seeks to be a "Bell lablet," to perform functions only a Hub can do, have an agile and dynamic structure, and serve as an integrated focal point for solar fuels. Its mission is to build an actual artificial photosynthetic system. Its 10-year goal is to demonstrate a scalable solar-fueled generator made from Earth-abundant elements that robustly produces fuel from the sun 10 times more efficiently than do crops. JCAP will cover from the macro to the micro scales.

The team has identified key information gaps: Earth-abundant light absorbers and photocatalysts; Earth-abundant, low-overpotential and efficient catalysts; photoelectrochemical membranes; a system for the integration of components; methods to understand and control the emergent phenomena on the mesoscale; and scalability and sustainability.

The Center has several principal investigators (PIs) drawn from institutions across the country. It has one building at LBNL and one at Caltech and a startup-company-like organization. Managers develop a budget and make sure the work gets done. There are a few things to be done: absorb light and produce more than 1.23 V. New material combinations are needed. For the part that is oxidatively stable, there are no materials available. Membranes need to be developed and oriented.

The Center is focusing on inorganic catalysts because robustness is needed. The historical rate of catalyst discovery for solar fuel reactions is too low. Earth-abundant, robust, inorganic light absorbers with optimal band gaps are needed.

In each research direction, every project has a definite starting point, goal, and method of accomplishment. The team has developed methods to characterize and screen 3 million materials a day. Data will be fed back to theorists. Only certain catalysts will be attachable to surfaces. Such materials will be screened for. Theory and ultrafast screening will be used. Advanced methods will be used to screen materials in 1 day rather than 5 years. Catalysts will be benchmarked under standard conditions so they can be compared.

[4] Dr. Lewis' full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

These pieces then need to work together rather than to destroy each other. Mesoscale membranes need to be identified. The formation of bubbles of fuel blocks the light, so using vapor rather than liquid water simplifies the problem. Rate constants from the macro to the micro scales will be determined by hardware prototyping.

There will be a focus on cost-cutting capabilities, and the Center will be an integrative influence. Flexible adaptive decision making will take the center where the science leads. Successful people will be given a new challenge. Such agile operations will result from constantly monitoring external developments, producing a monthly "hot list," rolling up a quarterly "hot list," and writing comprehensive annual state-of-the-field reviews.

The JCAP South facilities will be built on the Caltech campus; the JCAP North facilities will be built on the LBNL campus. The facilities will have DOE's EVO [Engineering Virtual Organization] video/audio links in all seminar rooms, offices, alcoves, and laboratories with a life-size tele-presence in selected meeting rooms (the virtual lunch room).

JCAP has a Science Advisory Board and a Strategic Advisory Board. The impacts of JCAP are focused on developing a commercially viable artificial photosynthesis technology. It will be a true "Bell-lablet": accelerate the rate of discovery; be an integrative center; serve as a unique focal point; and be an agile, dynamic scientific leader. In summary, JCAP will be a focal point to move artificial fuels forward, integrating current investigations and feeding challenges back to the scientific community.

Dr. Lewis answered questions posed by the panel.

Question: How much of Kansas would have to be covered with JCAP's system?
Answer: An area 100 km × 100 km would power the United States with electricity and fuel if equipped with a system operating at an efficiency of 10%.

Question: How can the East Coast could be involved with the hub?
Answer: Send students to the existing facility out West. Also, videoconferencing will glue together institutions in different locations with different cultures.

Question: The hub is targeting liquid fuels. Would it not be more effective to focus on nonliquids?
Answer: Success is not making a liquid fuel. The secret is to make *a* fuel. It is known how to convert one fuel to another. "He who cannot store will be powerless after 4 (pm)". Energy has to be stored, and that is easily done in liquid forms. The ultimate storage solution is in chemical bonds. There is nothing better than chemical bonds for energy density.

A break for lunch was declared at 12:02 PM.

Thursday, August 5, 2010
Afternoon Session

The meeting was reconvened at 1:22 p.m. **William Barletta**[5] was asked to report on the Compact Light Sources Workshop, the second in a series of workshops on photon sources.

[5] Dr. Barletta's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

The charge to the workshop was

- evaluate alternatives to canonical light sources that are becoming increasingly costly;
- examine the state of the technology of compact light sources (CLSs) and expected progress in emerging technologies; and
- identify advantages and disadvantages of CLSs relative to third-generation storage rings and free-electron lasers (FELs).

While CLSs would not substitute for large synchrotrons and FELs that typically incorporate extensive user-support facilities and provide beams of the highest quality, they do offer several advantages. A CLS would be university size in scale, taking up a few hundred square meters of floor space, costing a few tens of millions of dollars, operating for a few million dollars per year, and being easily expandable.

Scientific and technological vitality of X-ray science depends on access to facilities. CLSs offer attractive capabilities complementary to the large user facilities and are expected to produce an impact on a broad range of science and technology:

- small fraction of the cost and size of large national user facilities;
- rapid turnaround for high risk research;
- rapid advance in source technologies;
- personnel (i.e. students, scientists) with versatile capabilities;
- potential for technological and commercial applications and for the source to be taken to the application.

On a decadal timescale, CLSs offer the potential for a new paradigm of national user facility.

Other important conclusions noted in Dr. Barletta's presentation include:

- Within 5 years, R&D could produce infrared laser systems delivering kilowatt-class average power with femtosecond pulses at kilohertz repetition rates.
- With an inverse Compton scattering source, the electron beam has a greater power than the photon beam in a collision between a relativistic electron and a photon.
- At the low end of high-harmonic generation driven by femtosecond lasers is a low-cost, stand-alone, table-top-scale, tunable extreme ultraviolet (EUV/XUV) source with full spatial and temporal coherence and ultrafast pulse duration.
- At the high end, there is the high-peak-power XUV facility. A pulsed wave high harmonic generation (PW HHG) facility would deliver pulses in the XUV with parameters very similar to the FLASH FEL at DESY (Deutsches Electronen Synchrotron Laboratory, Hamburg, Germany) for a very modest investment
- Tabletop soft x-ray lasers (SXRLs) have a high pulse energy, a high average flux, one to three optical tables, full phase coherence, and a short pulse.
- Compact repetitive laser-pumped plasma soft X-Ray Lasers (SXRLs) have a wavelength range of 10 to 50 nm, an average power up to 20 μW, a pulse energy up to 10 μJ, a narrow spectral bandwidth, and a repetition rate from 1 to 10 Hz (possibly 100 Hz in the future).
- Discharge-pump lasers produce coherent average power at 46.9 nm, similar to synchrotron beam lines. Their average power is more than 1 mW; the pulse energy is 0.01 to 0.05 mJ.
- A potential breakthrough is a source based on plasma accelerators for an acceleration of 10 to 100 GeV/m operating at terahertz to megahertz synchronized to a couple of femtoseconds.

- In a laser plasma accelerator facility, the linac cost is minimal. As laser costs decrease and performance increases, each beamline could have its own laser.
- In plasma accelerators, seeding technology and accelerator technology are both advancing.
- Small storage rings are attractive. While not exactly compact, they might be better described at "chubby." New lattice designs and more compact magnets enable a reduction in size, a lowering of cost, and a facility that could offer 20 to 40 beamlines with the same flux and same brightness as bend-magnet beamlines at third-generation rings.

Dr, Barletta answered questions posed by the panel.

Question: Is the report on the BES website?
Answer: Not yet.

Question: Is there anything in laser light-source technology that the consumer community might become interested in to drive costs down?
Answer: The workshop looked at that. There is a divergence in users. This is an area that DOE will have to look at. It might be ripe for SBIR funding.

Question: Are these open user facilities rather than national user facilities.
Answer: Yes.

Question: Have you looked at whether current large-facility users might want to transfer to these smaller facilities thereby making room for additional users at the larger facilities?
Answer: No. Only capabilities have been looked at. These machines will not match the larger facilities' capabilities.

Paul Alivisatos[6] was asked to report on the Carbon Capture Workshop.

Stemming carbon dioxide emissions is a daunting challenge. Global energy use releases 37 gigatons of carbon dioxide to the atmosphere each year. The Energy Information Administration projects that global electricity generation will have a continued reliance on carbon-based fuels. Strategies that reduce carbon dioxide emissions call upon carbon capture, and an intermediate-stage technology will be needed for decades or centuries.

The workshop was asked to look at three scenarios:

- post-combustion,
- pre-combustion, and
- oxycombustion.

Current carbon capture technology works by concentrating the carbon dioxide by absorbing it into an aqueous amine solution, heating that solution to high temperatures, and boiling off the carbon dioxide. A lot of energy goes into this heating.

The scale of the problem is that a typical 550-megawatt coal-fired electrical plant emits 2,000,000 ft^3 of flue gas per minute. The scale is so large, and the concentration of CO_2 is so small (12%-

[6] Dr. Alivisatos' full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

14%) that it is costly to implement a control strategy. The cost of carbon capture today is $80 per ton or 8 cents per kilowatt hour. It causes a parasitic energy use of 25 to 30%.

Few energy technologies are so far off from the achievable limits. There is a real opportunity here. The carbon capture problem provides inspiration for deep new basic science. Nanoscience opens up new opportunities to tailor materials for carbon capture: liquids, membranes, and solids (and funny hybrids of these states). There is a challenge to design complex new interactions using architecture, shape, controlled binding, new triggers, and new approaches to cooperative binding.

Carbon dioxide can be pushed into a liquid. Adjusting the isotherms controls the rate of release. Could complex fluids be used? The gas–liquid interface controls the kinetics. The development of ionic fluids could substitute for energy or both enthalpy and entropy might be used for separations. Volatile solvents and chemistries include intermolecular interactions of gases dissolved in liquids, new chemistries and systems, and non-ideal absorption. There are some systems that normally are fluids and, under the influence of carbon dioxide, become ionic liquids. Membranes might be developed to act as carbon dioxide sieves.

There is a lot to learn from nature, which separates oxygen from air and combusts it at one temperature. Protein cages with enzymes inside might act as valves on carbon dioxide flow through a system. There is continuous innovation in the control of pore structure and connectivity, dimensionality, symmetry, and adsorbate-site interactions. Solid adsorbents may provide tunable structures. One can mix and match components on the nanoscale for new synthetic approaches for 3-D-nanoscale-membrane and solid-sorbent materials, including self-assembly. And one can exploit cooperative phenomena by designing materials in which carbon dioxide absorption and desorption would result in structural or chemical changes in which the resulting process is more thermo-neutral, alleviating the energetic penalty. One might also be able to design materials that react reversibly with molecular or ionic species. Selectivity membranes may be tuned with functional components, and target molecules might be selectively transported across membranes with new mechanisms made up of nanowires or some such. Polymeric membranes may hold promise for separating carbon dioxide with (for example) polymer-peptide block copolymers.

Carbon capture is a really important problem to work on. Without it, carbon dioxide levels cannot be brought down.

Dr. Alivisatos answered questions posed by the panel.

Question: Does nature uses photons to create a trigger?
Answer: Yes.

Question: How many acres of algae it would take to absorb all the carbon dioxide.
Answer: With 10% efficiency of algal pickup, 2% of all land area would be required. The efficiency of algal pickup is more like 0.3%, so the required area would be huge.

Question: How many gigatons of carbon dioxide are absorbed by the ocean?
Answer: About a quarter of a gigaton.

Dion Vlachos[7] was asked to review the highlights of the Catalysis Center for Energy Innovation.

[7] Dr. Vlachos full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

The Catalysis Center for Energy Innovation (CCEI) consists of 22 faculty researchers from 9 academic institutions with a variety of expertise. The Center's mission is to:

- develop the enabling science leading to improved or radically new heterogeneous catalytic technologies for viable and economic operation of biorefineries from various lignocellulosic biomass feedstocks;
- educate the workforce needed to further develop and implement these two technologies; and
- pursue technology transfer via multi-institutional collaborations and joint ventures with industrial partners.

The three major research goals are to:

- transform biomass and/or its derivatives into valuable chemicals, fuels, and electricity through a fundamental understanding of the chemistry and catalyst performance;
- design novel hierarchical multiscale materials with nanoscale resolution suitable for processing derivatives from complex, multiphased media of biomass to ensure efficient, highly selective, and benign processes; and
- promote catalyst design and technology advancement of novel theoretical and multiscale simulation platforms and cutting-edge characterization tools.

The grand challenges are:

- Lignocellulosic biomass decomposition leads to coking and is slow.
- The complex feedstock renders fundamental studies difficult.
- Processing of biomass derivatives occurs in a complex environment.

The research thrusts include: chemicals, fuels, and electricity, with four different approaches:

- hierarchical multiscale materials;
- multi-scale modeling;
- characterization techniques; and
- cross cutting research.

In its first year, CCEI developed a novel catalyst for the single-pot conversion of glucose to 5-hydroxymethylfurfural (HMF), developed a computational engine for model-based bimetallic catalyst discovery applied to reforming technologies, defined surrogates of bio-oil, and investigated molten-metal-electrolyte-based fuel cells for the direct conversion of carbon to electricity.

Dr. Vlacos discussed the Center's work using Sn-beta zeolitic catalysts to isomerize glucose in water and for coupling upstream (hydrolysis) and downstream (dehydrogenation) with glucose isomerization reactions. Computations were used to complement experimental work.

The conclusions are that

- A large-pore zeolite that contains tin is able to isomerize glucose to fructose in aqueous media with high activity and selectivity.
- The same reactivity is achieved when a highly concentrated glucose solution is used.
- The catalyst can be used for multiple cycles without regeneration.
- The catalyst is able to perform the isomerization reaction in highly acidic, aqueous environments with equivalent activity and product distribution as in media without added acid.

- The catalyst is able to perform Lewis-acid-mediated isomerization of glucose in pure water solvent or saturated NaCl solutions.
- “One-pot” synthesis of HMF from glucose with high-yield is possible.

Dr. Vlachos answered questions posed by the panel.

Question: Over what range of pH does this work?
Answer: Very low pH: 1 to 2. The next step is to move away from homogeneous catalysis.

Question: Do you get any net energy from this process?
Answer: Yes.

Question: How quickly after a discovery is made does the new information get disseminated to the rest of the researchers and affects their research?
Answer: Within a week. Teleconferencing can be used to disseminate information.

Question: How is intellectual property is handled?
Answer: They file for patents. Discussions about the research are recorded, and sometimes the IP is owned by two or three institutions.

Question: There is a vast industry making high fructose corn syrup. Could industry use this catalyst instead of enzymatic conversion?
Answer: The fructose could go to foods or to fuel. This Center focuses on fuels.

Question: How does the Center’s activity lead to the insights and key experiments?
Answer: The Center promotes lots of discussions that produce new ideas.

A break was declared at 3:02 p.m. The meeting was called back into session at 3:20 p.m., and **Alex Malozemoff**[8] and **John Sarrao** were asked to present the report, *Science for Energy Technology: Strengthening the Link Between Basic Science and Industry*[9].

Chairman Hemminger thanked Alex Malozemoff and George Crabtree for the tremendous amount of work they devoted to this project. In setting up the workshop, areas were down-selected, and some energy-related areas were not covered. Who is the audience of this report? The short, concept report’s audience was DOE upper management and the Washington policy community. This report is aimed at BES, SC, and the scientific community.

Dr. Malozemoff said that the charge to the Subcommittee was to

- summarize the basic research needs (BRNs) themes;
- identify the grand-challenge science drivers that are likely to have an impact on energy in the near term;
- identify how BES user facilities can impact basic and applied research on energy; and
- identify major impediments to achieving transformative energy technologies.

[8] Alex Malozemoff and John Sarrao’s full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

[9] The full report is available at: http://www.er.doe.gov/bes/reports/abstracts.html#NGPS

Two reports were to be produced: a short concept report and a detailed technical report. The SciTech Workshop was held January 18-21, 2010, with about 100 participants from industry, the national laboratories, and academia. It had panels on major energy topics and the use of facilities. Each panel identified PRDs and nontechnical barriers. Industry interaction with basic scientists was a highlight of the workshop.

The 15-page concept report was approved by BESAC in April 2010. The full 200-page report is presented at this meeting for discussion. It repeats and amplifies the main themes of the concept report. Many opportunities exist for BES science to make a transformative, near-term impact on the nation's energy problems. To do that, direct collaboration with industry is important, and BES scientific user facilities can play a major role in this process.

The technical motivation for reaching out to industry is that innovation is needed. Clean energy technologies operate far below their theoretical potential. Often, the industry roadblock is a basic science understanding of materials, chemistry, and energy conversion at the nanoscale. Another reason to reach out is that there are some challenges, and the nation needs jobs in new technologies. Industry is the vehicle for commercialization. This is an urgent issue. Other countries are starting to take the lead in establishing clean-energy technology. Other parts of the U.S. R&D enterprise are starting to move into the science-to-industry space. BES is best positioned to address the needs with its huge expertise base, but the window of opportunity is narrow.

The BRNs have already identified two kinds of science contributions to energy: (1) discovery-driven science that produces breakthroughs and (2) understanding and ultimately controlling existing phenomena. Transformational near-term research is not an oxymoron because discoveries eventually cross the economic tipping point.

There are three overarching themes of the report:

- Develop foundational scientific understanding of at-scale production challenges in existing materials and processes.
- Develop a fundamental understanding of the lifetime prediction of materials in extreme environments, especially aging, degradation, and failure.
- Discover new materials or chemical processes with targeted functionality and shorten the timeline on their development.

Three crosscutting needs are seen:

- new materials by design with specific properties or functionalities;
- understanding, predicting, and controlling interfaces; and
- dynamic behavior away from equilibrium.

The concept report was presented to Drs. Brinkman, Koonin, Dehmer, Kung, and House and Senate staffers. There was positive feedback, but action awaits the full report.

Sarrao said that PRDs were identified for each of the eight panels. The SciTech workshop PRDs complement the BRN PRDs but have different foci. In harnessing solar energy with photovoltaics, the opportunity is that sunlight can supply a large fraction of the world's energy needs. The problem is that the most promising converter of photons to electricity needs a halving of its cost and an increase in its efficiency when produced at the commercial scale.

In carbon dioxide sequestration, the opportunity is to isolate carbon dioxide in underground sites to enable clean use of fossil fuels. The problem is that one must understand the site capacity and the ability to inject and contain carbon dioxide and be able to assure sequestration for thousands of years.

In superconductors for a high-capacity grid, the opportunity is efficient long-distance transmission of renewable energy. The problem is that superconductors carry one-tenth the current that theory says they could.

In solid-state lighting, the opportunity is to save 22% of today's entire electricity use. The problem is that, again, there is a huge drop in performance as one goes from the laboratory scale to the manufactured model.

BES user facilities have unique resources for probing structure, spectroscopy, and imaging and for nanoscale synthesis and characterization. They hold a high value for the industrial user base. The workshop identified four recommendations for user facilities:

- Enhance industrial outreach and develop a systematic and sustained effort to engage targeted industrial sectors.
- Review and modify existing user-facility access policies and priorities.
- Take advantage of current capabilities.
- Push the limit of future capabilities for high spatial, spectral, and temporal resolution to meet increasingly sophisticated measurement needs for discovery and development of next-generation energy systems and technologies.

The last chapter of the report focuses on barriers and solutions. Barriers to communication are differing objectives and styles. The workshop formed a promising opening:

- BES needs to reach out to advisory boards and form personal relationships.
- For collaboration, challenges must be found that exploit basic science to advance industrial performance.
- Consortia should be formed for common problems.
- Academia–national laboratory–industry exchange programs should be established.
- Intellectual property needs a case-by-case solution and the recognition of the legitimate needs of both sides.
- The workforce challenges are to establish collaborative research projects, student and postdoctoral internships in industry, and exchange visits across universities and national laboratories and industry.

The first round of feedback from Committee members has already been incorporated in the full report, and follow-up activities need to be identified.

Following their presentation, Drs. Malozemoff and Sarrao addressed comments and answered questions from the panel.

Comment: Many of these PRDs were vague, and that is how they were desired to be so the commercial and BES people could work together.

Comment: The report is vague. A researcher looking for ideas for new research opportunities will be frustrated. What should be figured out is what has to happen before collaborations are started. The BES researcher needs to know enough to be valuable. Younger PhDs need to be gotten into industry. The BES community has to become familiar with industry to be able to pose research opportunities. The report is too long. There is a lot of redundancy that could be eliminated. The report could be reduced by one half.

Comment: It was revealing to hear what the people from industry were talking about. Collaborations with industry would have to be based on such discussions. Regarding the length of the report, some things can be put into supplements or appendixes. The people who came from industry did a great job, and BES and BESAC should be thanking *them*.

Comment: The chapter on user facilities underpins the desire to establish collaborations. Less than 5% of the light-source usage and less than 1% of the neutron-source usage is by industry. There should be reasons offered in the report for the sharp decline in industry usage at the user facilities. While the user community at large has doubled, industry users have not doubled. But the reason has not been identified. There has been a subset of industrial users at any facility that has been there since the very beginning. Why other companies do not participate is not known. One needs to explain to industry how to scale from short exposures to sizable radiation exposures. One has to be willing to invest in these long-term experiments.

Chairman Hemminger observed that this had been a far-ranging discussion. The general tone had been that the Committee likes the report. A number of comments about follow-ups could be made. He suggested that the Committee think about it overnight and revisit the issues on the following day. It could also accept the report with advice for updating it. He asked for a motion.

Dr. Greene moved to accept this study with the friendly amendments recommended by the Advisory Committee being considered seriously and incorporated where possible, particularly those on paper and web readability. Dr. Tobias seconded the motion. Dr. Hemminger stated that it would be interesting to make a web version that was very navigable.

Dr. French asked whether the vote was strictly to accept or not to accept. Chairman Hemminger said that, ultimately, the Committee has to accept the report or reject it. The Committee also has to forward some recommendations to BES. That advice should not be too prescriptive and should not tie BES's hands.

The question was called, and the motion passed unanimously. Chairman Hemminger said that the Committee would broaden the discussion on the following day to include what could be done to move the issue down the road. The floor was opened to public comment.

David Miller said that the Office of Nuclear Energy (NE) should support the Advanced Test Reactor (ATR) at Idaho National Laboratory for material testing by industry.

Gregory Exarhos expressed appreciation of Dr. Richmond's report. He was disheartened by Congress's cutting the funds for the SC Graduate Fellowship Program. The need for graduate-student support should continue to be a priority.

There being no further public comment or Committee business, the meeting was adjourned for the day at 5:09 p.m.

Friday, August 6, 2010

The meeting was called to order at 8:59 a.m. by Chairman Hemminger. He reviewed the agenda and introduced **Harry Atwater**[10] to present highlights from the Energy Frontier Research Center (EFRC), "Light–Material Interactions in Energy Conversion."

The scientific vision of the Light–Material Interactions in Energy Conversion Project is to tailor the morphology, complex dielectric structure, and electronic properties of matter to sculpt the flow of sunlight and heat, enabling the conversion of light to electrical and chemical energy with unprecedented efficiency. Its goal is to create a national resource for fundamental optical principles and phenomena relevant to solar energy conversion, and for the design of the optical properties of materials and devices used for energy conversion. It is focusing on manipulating light. It combines the disciplines of electromagnetic theory, plasmonics, metamaterials, materials physics and chemistry, and applied mathematics (algorithms). The capabilities it employs include 3-D nanolithography, 3-D nanostructural synthesis, colloidal nanostructures, light-driven structure design, and complex architectures. Bringing these disciplines together should produce light trapping and spectrum splitting beyond the classical limit, light focusing for efficient energy conversion, and probing extremes of spontaneous emission and absorption.

The initial 5-year research directions include:

- design of an optical system capable of visible and ultraviolet light generation from sunlight using cooperative upconversion;
- definition of the limits to absorption and spontaneous emission;
- establishing fundamental transformation optics principles for light absorption and emission in complex metamaterial structures; and
- developing light-driven material-synthesis processes. The center activities focus on graduate and postgraduate research, unique facility and bench top technique development, researcher workshops, an energy-science seminar series, broader communications, and mentoring of young scientists.

There are four research groups.

- The research group on Visible and Ultraviolet Generation by Upconversion is designed to develop materials and structures that enable efficient upconversion of the solar spectrum.
  - Absorbed photons of a given frequency can be converted into higher-harmonic photons through cooperative upconversion. Rare-earth oxides do this.
  - This research is conducted with fiber-coupled high-Q resonator characterization.

- The research group on Metal Optics for Spontaneous Emission and Absorption Enhancement is designed to explore limits to optical absorption and spontaneous emission in metallodielectric materials.
  - Develop principles for design of ultrathin photovoltaic absorbers with nanoscale dimensions; and
  - Manipulate local density of states in metallodielectric structures to control spontaneous emission. It is interested in making materials for thin-film photovoltaics.

[10] Dr. Atwater's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

- The third research group, Transformation Optics for Photovoltaics, is designed to study methods for transforming a physical space into a desired virtual space.
    - The transformation is equal to coordinate transformation and results in spatially varying material properties within a transformed region.
    - In the third research group, researchers are using 3-D interference lithography, in which a mask produces interferometry that produces the desired pattern.

- The fourth research group, Self-Architected and Complex Architecture Absorbers, is designed to tailor light absorption and dielectric materials with complex architectures and to develop light-driven material-synthesis processes that enable materials to develop architectures in response to illumination.

Transformation optics is an exciting topic for electromagnetic theory. The desire is to enhance performance and minimize absorption by spatially varying the dielectric function. One can then build something that varies the refractive index. An example of this work is the Luneburg lens solar concentrator that has a refractive index of 1 at its surface. A radial variation is induced to achieve focusing. It is difficult to integrate the spherical shape and to manufacture the radially varying index. The manufacturing solution is to photo-electrochemically etch silicon directly from an image produced by an algorithm.

Another initiative is to design a metamaterial layer that can efficiently couple the solar spectrum into a thin-film solar cell. This would form a perfect absorbent that has no reflection and is insensitive to the incident angle and wavelength of light. A plasmonic metamaterial has been developed that is polarization insensitive, is angle insensitive up to 50°, and is tunable with frequency. For more complex coupling schemes, one can locally modify the metamaterial effective index. With such a structure, one can modify the refractive index by etching valleys in the surface.

The center uses facilities at the University of Illinois at Urbana, Caltech, and LBNL. Team communications are carried out with videoconferencing, team meetings, and a wiki. A 3-D nanofabrication workshop was held on March 24-25, 2010, in Urbana, Illinois. An EFRC workshop was held July 7, 2010, in Pasadena, California. Workshop lectures are online.

In summary, the center is up and running and fully operational. PIs, post docs, and graduate students are in steady state. Three internal review team meetings and one workshop have been held. There is a focus on team communications. Research is well under way, and connections are being developed with other centers and institutions.

Following his presentation, Dr. Atwater answered questions posed by the panel.

Question: Have you looked at reflective optics?
Answer: There is a lot of research on black holes, which are perfect absorbers. One can use photochemical etching to funnel the light into the material.

Question: Are there any inroads in teaching of electromagnetic theory?
Answer: This is often the province of electrical engineers, but Atwater required all of his students to take a course in the subject.

Janos Kirz[11] was introduced to report on the COV of the Scientific User Facilities Division of BES, the largest division of BES in terms of funding.

The COV looked at light sources, neutron sources, nanocenters, electron microscopy centers, accelerators and detectors, and construction projects. It concluded that proposal review and recommendation processes were excellent, as were the processes to monitor and review active projects. The award processes continue to enhance the breadth and depth of portfolio elements as well as their national and international standing. The response by the Division to the previous COV report was excellent. Implementation of the recommendations has led to improvements of the process and documentation, and the Division staff has been increased.

The cooperation of the staff made the COV process very effective, although the timing of the COV coincided with an incomplete cycle of nanocenter reviews and dealing with paper files was less efficient than dealing with digital files would have been. Scheduling the COV to coincide with the cycle of nanocenter reviews and a brief update by a program manager cognizant of the facility type being reviewed would be useful.

The 3-year reviews of the facilities are well organized and well executed, and the review teams are carefully selected. The facility responses to the reviews' recommendations are uneven. Assessment targets used by the reviewers are not communicated to the facilities, which are then unprepared to address reviewers' questions. Terms like "high-impact journal" are not used in a standard manner, and reporting on off-site users is not uniform. Some reviews are overly long and detailed and therefore do not receive sufficient attention.

The COV recommended that as part of the 3-year reviews:

- the facilities should be asked how previous recommendations have been implemented;
- the facilities should be provided with the questions to be answered;
- reviewers should be drawn from a broader base than the national laboratories;
- publications and off-site users should be uniformly defined; and
- reviewers should be asked to summarize major findings and recommendations at the beginning of their reports.

The COV commended the Division for recognizing the importance of supporting staff research and the selection of high-quality scientists. Different facilities serve different communities, and they are all needed and important. The COV commended BES on its recognition of the importance of the tools provided at the user facilities and the people who oversee those tools.

Today, fewer users are well trained in the operation of beamlines, end-station equipment, and data acquisition. The COV recommended that the areas of experimental apparatus, sample environment, and software receive added emphasis. Additionally, the the COV recommended that the Division's travel budget and office space should be increased; facilities should prepare an annual list of publications and currently available equipment; a pipeline of instrumentation, accelerator, and detector experts should be fostered; and more outreach should be developed to train users in the use of the facilities.

Following his presentation, Dr. Kirz responded to questions and comments posed by the panel.

[11] Dr. Kirz's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

Question: Is there any progress in the transition from paper to electronic files?
Answer: It varies by division. Dr. Montano added that everything is in electronic format, but for several reasons is transferred to the COV in printed form.

Question: Did the COV look at safety procedures at the facilities?
Answer: The COV did not look at safety per se. A lot of attention is paid to safety at the facility level, and the facilities operate safely.

Comment: The recommendation for the provision of theory support at scientific facilities was appreciated. That recommendation might be implemented by incorporating theory groups into the Computational Materials and Chemistry for Innovation report that is currently under development.

Question: Is there a systematic effort to identify aging equipment and infrastructure and to decommission the out-of-date infrastructure?
Answer: Kirz responded that the facilities that he was familiar with are interested in updating aging elements, but it is easier for them to get new instruments.

Chairman Hemminger asked for a motion to accept this report. Dr. Gates moved to accept the report, and Dr. Cummings seconded the motion. It passed unanimously.

Under Secretary Steven Koonin[12] was introduced to provide an overview and perspective.

Dr. Koonin began by thanking the members of the panel for their service and commitment. He noted that DOE has four missions:

- to sustain basic research for the discovery potential and to support the Department's missions;
- to catalyze the transformation of the national and global energy system;
- to enhance nuclear security; and
- to contribute to U.S. competitiveness and jobs both long-term and near-term.

The United States has been a global leader in basic research for 50 years. But now the rest of the world is investing a lot of money in science. It is unclear if the United States is still the leader in many fields. DOE needs to balance resources in basic research between fields that are close to application versus those distant from application. Agencies must talk to the public and to Congress more effectively. Climate science must be improved. It has gone from an academic exercise 30 years ago to prominence today. Dealing with these issues is a major priority of the Department.

Concerns about energy security and reducing greenhouse-gas emissions are the drivers for energy transformation. To enhance energy security, the target is to reduce crude-oil use by 3.5 million barrels per day. To check greenhouse-gas emissions, a 17% reduction in emissions is sought by 2020 and an 83% reduction by 2050. Changes in energy supply occur at decadal scales. It takes a long time to make changes in energy use.

One question is how to hook up science and technology with society and industry. The government does not operate the major energy enterprises in the country. Another question is what are the best research structures? Coupling basic and applied research is being addressed

[12] Dr. Koonin's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

with the energy hubs and ARPA-E. The policy must be gotten right because a reliable and enduring policy must be in place before industry will move.

Nuclear security is half the energy enterprise. DOE must maintain a technical base. It must keep its staff engaged even though it is not testing weapons anymore. We need to exploit the simulation capabilities developed for simulating physical nuclear testing. In that regard, DOE will begin a sustained-burn campaign in a couple of weeks at the National Ignition Facility.

In U.S. competitiveness, a deep understanding of the issues must be grasped. The rest of the world is growing and developing faster than the United States. The long-term trends in domestic output and employment are not in the nation's favor. Scientists and science and technology must determine the right strategy and what roles they are to play. Innovation is key to competitiveness.

Simulations expand scientific and technical understanding. DOE is providing petascale machines to the scientific community to work on biology, turbulence, nuclear energy, fusion energy, biofuels, and quantum chromodynamics. If one can simulate energy systems with high fidelity, one can optimize designs, compress the design cycle, and facilitate a transition to scale. The rest of the world is working hard in this area.

In FY09, federal spending was largely for Social Security, Medicare, Medicaid and the State Children's Health Insurance Program, unemployment and welfare, interest on the national debt, and the Department of Defense (DoD). DOE is in the discretionary portion of the budget. This is unfortunate because the federal deficit is shaping the budget discussions. There has been a phase shift that will cause financial discussions in the coming years.

Dr. Koonin concluded by again thanking the Committee for its hard work and continued dedication to advising the government. He then responded to questions and comments from the Committee.

Question: What kind of image, or lack thereof, does DOE have with the U.S. public?
Answer: The agency seems to be invisible. Catalyzing change in the Department's interactions with industry is important. The DOE Under Secretaries and the Secretary are working closely with industry. They are out and about speaking with industry. A dialogue is needed with industry about what basic research is needed. More workshops with industry would be good.

Question: A recent opinion piece in *Nature* said that involvement of DOE with the DOD and its contracting ability was necessary to move changes in the energy industry. Could you comment?
Answer: DOE has signed a memorandum of understanding with DOD in energy efficiency. For example, it takes 9 gallons of fuel to get one gallon of fuel to the front. So we need more efficiency. We hope to use their bases as testbeds for technology. They can also be the first buyers for alternative fuels. But DOD uses only 1% of the energy in the United States. The U.S. Government is only one customer. DOE must interface effectively with industry. This is very important, and very problematic.

Question: How can BES catalysis researchers can be encouraged to understand what the industry's needs are?
Answer: The only way is to get industry involved. For example, send a DOE lab researcher to an industrial lab for a year. Workshops and focused projects are other ways to inform researchers.

Question: Can the concept of a "research campaign" be used effectively by SC to do that?

Answer: Yes, but more than just in BES. It should involve the whole Department. And next week there will be a "dollar-per-watt" workshop involving people from across DOE.

Comment: This link between industry and BES has to be grown (e.g., through user facilities). But the future members of industry also have to be trained. BES's main role cannot be forgotten: fundamental research.
Response: The Under Secretary agreed that one has to strike a balance between basic and applied research. There is a whole other part of DOE (the applied-technology offices) to deal with industry. And connecting the Office of Science people with the DOE applied research people is as important as connecting with industry.

Alex Malozemoff and **John Sarrao** were asked to comment further on the SciTech workshop report. Sarrao said they would incorporate many useful "minor" suggestions and would format an online version for accessibility and ease of reading. They will move Barriers and Solutions from Chapter 11 to Chapter 2, address the "context" discussion, include an additional sidebar example, reach closure on the final cover art, and shift the focus to outreach and implementation activities. There will be changes to the Table of Contents, the Introduction, and Chapter 2, Barriers and Solutions. A new version should be ready in a matter of days.

Dr. Greene said that she supported this report as it stands. The Committee should go on to the next stages quickly. The report should be broken down into Chapters 1 and 2, it should be made readable, and it should be sent out to industry, Congress, foreign embassies, etc., and this Committee should move on to the next step.

Chairman Hemminger said that the Committee needs to think about how to organize these next steps and to stimulate the follow-on activities of BESAC and BES. He thanked the team for their hard work and diligence.

The floor was opened for public comment. Dr. Exarhos said that there are examples all around the national laboratories of shared postdocs. In some cases, the postdoc was ultimately hired by the industry in which he or she worked.

There being no further comment or business, the meeting was adjourned at 11:28 AM.

Respectfully submitted,
Frederick M. O'Hara, Jr.
Recording Secretary
August 26, 2010
(Edited 10/08/10, MIS)