Minutes of the
Basic Energy Sciences Advisory Committee Meeting
November 5–6, 2009
Gaithersburg Marriott Washingtonian Center
Gaithersburg, Maryland

BESAC members present:

Simon Bare
Nora Berrah
Sylvia Ceyer
Peter Cummings
George Flynn
Bruce Gates
Laura Greene
John Hemminger, Chair
Sharon Hammes-Schiffer
Michael Hochella
Bruce Kay
Kate Kirby (Thursday only).
William McCurdy, Jr.
Daniel Morse
Martin Moskovits
Kathryn Nagy
John Richards
Kathleen Taylor
Douglas Tobias
John Tranquada

BESAC members absent:

Sue Clark
Frank DiSalvo
Mostafa El-Sayed
John Spence

Also participating:

William Barletta, Director, United States Particle Accelerator School, Department of Physics, Massachusetts Institute of Technology
Peter Blair, Executive Director, Engineering and Physical Sciences Division, National Academy of Sciences
Linda Blevins, Senior Technical Advisor, Office of the Deputy Director for Science Programs, Office of Science, USDOE
William Brinkman, Director, Office of Science, USDOE
John Corlett, Head, Center for Beam Physics, Accelerator and Fusion Research Division, Lawrence Berkeley National Laboratory
Patricia Dehmer, Deputy Director for Science Programs, Office of Science, USDOE
Mary Galvin, Division of Materials Science and Engineering, Office of Basic Energy Sciences, USDOE
Linda Horton, Director, Materials Science and Engineering Division, Office of Basic Energy Sciences, USDOE
Harriet Kung, Associate Director of Science for Basic Energy Sciences, USDOE
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Katie Perine, BESAC Committee Manager, Office of Basic Energy Sciences, USDOE
Eric Rohlfing, Director, Chemical Sciences, Geosciences, and Biosciences Division, Office of Basic Energy Sciences, USDOE
Harold Shapiro, Professor Emeritus, Departments of Economics and Public Policy, Princeton University
Marvin Singer, Senior Advisor, Chemical Sciences, Geosciences, and Biosciences

Division, Office of Basic Energy Sciences, USDOE
Rachel Smith, Oak Ridge Institute for Science and Education
William Valdez, Director, Office of Workforce Development for Teachers and Scientists, USDOE

About 95 others were in attendance in the course of the two-day meeting.

Thursday, November 5, 2009
Morning Session

Chairman **John Hemminger** called the meeting to order at 8:31 a.m. Rachel Smith made safety and convenience announcements. The Committee members introduced themselves. **William Brinkman**[1] was asked to give an update on the activities of the Office of Science (SC).

Dr. Brinkman reviewed the DOE organization chart, and noted that DOE is divided into three sections: the National Nuclear Security Administration (NNSA), applied-technology offices, and the Office of Science (SC). SC interacts with many of the NNSA and applied-technology offices, such as Energy Efficiency and Renewable Energy (EERE), Fossil Energy (FE), Nuclear Energy (NE), and Electricity Delivery and Energy Reliability. Some of the important issues involving these other DOE offices include: deliberations on how to manage the NNSA laboratories; trying to revive nuclear energy and get it moving more in this country; and with respect to electricity, the smart grid.

Dr. Brinkman reviewed the Office of Science budget for FY 2010. We are on track to double the budget, and hopefully this will happen. For the first time in 11 years, he said, the Department of Energy (DOE) started the fiscal year with a budget. Actually, three budgets have been produced in the past year: FY09, American Recovery and Reinvestment Act (ARRA), and FY10. He noted that about one-third of SC's budget goes to Basic Energy Sciences (BES). Other major programs within SC are the offices of High Energy Physics (HEP), Nuclear Physics (NP), Biological and Environmental Research (BER), and Advanced Scientific Computing Research (ASCR).

SC's leadership goals and challenges are to maintain excellence and world leadership in its scientific programs; the planning, construction, and operation of its scientific user facilities; the management of its 10 DOE national laboratories; and the management of its federal and contractor workforces. We have been developing new approaches to integrate basic and applied research to address the challenges of energy technologies. These include establishing Energy Innovation Hubs, using lessons learned from the three Bioenergy Research Centers (BRCs) and the 46 Energy Frontier Research Centers (EFRCs). In addition, the Department has established ARPA-E

The BRCs are revolutionizing the discovery of future energy solutions with a focus on feedstock characterization and development, feedstock deconstruction, and feedstock conversion to liquid fuels. These BRCs (the Joint Bioenergy Institute, Great Lakes

[1] Dr. Brinkman's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

Bioenergy Research Center, and BioEnergy Science Center) have been quickly initiated and are making rapid progress.

Forty-six EFRCs were awarded $777 million over five years. Those centers represent 102 participating institutions in 36 states and the District of Columbia. Three Energy Innovation Hubs were appropriated in FY10: Fuels from Sunlight (SC lead), Energy-Efficient Building Systems Design (EERE), and Modeling and Simulation for Nuclear Fuel Cycles and Systems (NE). The "one roof" reference in the appropriation refers to real leadership with budgetary authority.

SC has started the Office of Science Graduate Fellowship Program to support outstanding students pursuing graduate training and basic research in areas of physics, biology, chemistry, mathematics, engineering, computational sciences, and environmental sciences relevant to SC. The program began accepting applications for the FY 10–11 academic year on September 30, 2009. ARRA funds ($12.5 million) will fully support approximately 80 fellowships. FY 10 appropriated funds will support approximately 80 additional fellowships in the program's first year.

All energy sources are evolving. This leaves us with a set of "energy imperatives", including: increased energy efficiency; increased use of renewables; increased use of carbon capture and sequestration (CCS) technology; increased nuclear power; and improved climate prediction. The National Academy of Sciences' (NAS) report, *America's Energy Future*, said that there is no technological "silver bullet" at present that could transform the U.S. energy system. Such transformation will require a balanced portfolio of existing (although perhaps modified) technologies, multiple new energy technologies, and new energy-efficiency and energy-use patterns.

SC's approach to these imperatives is multipronged, and includes:

- increasing combustion efficiency using ultrafast imaging of fuel and biofuel sprays;
- increasing combustion efficiency through advanced gas sensors which can provide real-time tuning and balancing of combustion burners;
- using X-ray studies to understand the performance of Pt-Cu catalysts in polymer electrolyte membrane fuel cells (PEMFC);
- studying commercial batteries in action with X-ray diffraction;
- using X-ray diffraction to characterize and optimize solar cell processing and materials; and
- investigating natural photosynthesis to gain new insights into the water-splitting mechanism.

This year's chemistry Nobel Prizes is based on X-ray crystallography, and the seminal work for this prize was conducted at DOE light sources with support from the Office of Science and from the National Institutes of Health.

Dr. Brinkman answered questions posed by the panel.

Question: Is there a scientific effort to understand the causal relationship between the increase in CO_2 and the decrease in ice mass?
Answer: That this is one of the things that the Office of Science is trying to address by building better models and enhancing the measurements. More SC money is being put into modeling. The National Aeronautics and Space Administration (NASA) has to step up and put more satellites into space. The GRACE satellite will die in 2012 or 2013.

Question: Is the fuels-from-sunlight hub was going to cover the Berkeley work?
Answer: This is part of another center at Berkeley. The hub will be funded separately.
Question: Has the Office of Science surveyed the entrepreneurial results that have come out of BES research?
Answer: There have been 173 startups in solar cells, and large companies are selling about 1 GW per year in solar equipment and have produced great improvements in the cost per kilowatt. These enterprises have resulted from a variety of funding sources. It is an important point that successful commercial ventures come out of BES research.

Question: What is the timescale for adding ultrafast light sources?
Answer: As soon as possible.

Question: For years, it has not been recognized that DOE/BES is the largest funder of science in the United States. This year, the focus on energy research by the leadership is remarkable and could change the public image of DOE. What is being done to change that public image? NASA advertises what it does on the web, TV, etc.
Answer: The Secretary is on an enormous public campaign to raise the issue of energy relative to science and applications. He is changing the perception rapidly. The Department is getting noted in presidential speeches. People no longer question the Department's right to do research. However, the fact that it is one of the largest funders of science in the United States still needs to be sold.

Harriet Kung[2] was asked to review the activities of the Office of Basic Energy Sciences (BES).

Dr. Kung noted that BESAC has been involved in strategic planning activities that have plotted a visionary path forward in a variety of sciences. Society needs to transition from traditional energy sources to sustainable energy materials. This opens a new era of science at the atomic and molecular levels.

A sustained effort is needed in research and scientific-tool development. Three modalities of research supported are:

- Core research, which supports single-investigator and small-group projects to pursue their specific research interests to spur future researchers and research.
- EFRCs, which are $2- to $5-million-per-year research centers, established in 2009, focused on fundamental research related to energy in certain areas to accelerate the development of next-generation energy sources.

[2] Dr.Kung's full presentation is available at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

- Energy Innovation Hubs, which are $20 million-plus per year research centers that will focus on integrating basic and applied research with technology development to enable transformational energy applications, combining scientific push and commercial pull in one place. Three hubs were approved, including SC's fuels from sunlight, in which BES has had a long-standing interest.

There are two main limits to solar fuel production: high capital costs, and fuel storage. Needed are photovoltaic cells to produce current that is fed to an electrolyzer to provide hydrogen gas. The ultimate goal would be direct conversion (e.g., through solar microcatalytic energy conversion). But, chemists do not yet know how to photoproduce O_2 and H_2, reduce CO_2, or oxidize H_2O on the scale needed. There is a huge gap between current capabilities and the technical goal. What is needed to be understood is:

1. Photon absorption and harvesting (i.e., How does one control light harvesting to utilize all of the photons?)
2. Charge separation and transport (i.e., How does one avoid recombination of photo-generated charge carriers?)
3. Photocatalysis (i.e., How do we produce fuels with the energy provided by visible light absorption?)

If one looks at the readiness of the different steps, one finds that most are in their infancy. They are nowhere near a commercial solar fuel technology. This science needs to be pushed toward commercialization and industrialization.

Currently, a wide range of probes are supported at the light sources, neutron sources, electron-beam sources, and Nanoscale Science Research Centers. What is envisioned is a national strategy for light sources. Those facilities have to be looked at in a capacity mode as well as in a capability mode. The Advanced Light Source, Advanced Photon Source, National Synchrotron Light Source (I and II), and Stanford Synchrotron Radiation Lightsource will be very useful tools for 10,000 to 15,000 users per year. Also needed are high-brightness, high-coherence facilities (photon capability machines), which will entail the LCLS and also future fourth-generation light sources.

BES published the report *Next-Generation Photon Sources for Grand Challenges in Science and Energy* and conducted a workshop on Accelerator Physics of the Next-Generation Light Sources to ask the question, "What is the technical readiness of the options faced?" There is a new BESAC charge on science for technology. The co-chairs for the study are Alex Malozemoff (American Superconductor) and George Crabtree (Argonne National Laboratory). It will ask what types of changes can be expected and what support will be needed. The workshop will be held in January 2010.

Major BES accomplishments in FY 2009 include:

- The Energy Frontier Research Centers (EFRCs). Forty-six centers were awarded. These EFRCs need to be balanced with individual research efforts.
- Single-Investigator and Small-Group Research (SISGR) awards. A total of $55 million was awarded in FY09 for SISGRs. These include single investigator awards ($150,000 to $300,000 per year), small group awards ($500,000 to $1.5

million per year) for up to 3 years, and midscale instrument (up to $2 million). Ninety-five SISGRs awarded: 72 university awards and 23 national-laboratory awards directed toward grand challenge science, use-inspired discovery science, and midscale tools for 21st Century science.

- With the EFRC and SISGR awards, nearly all of BES's funding has been obligated. (The exception is the Early Career Awards.)
- The first X-ray laser in the world produced its first light on April 15, 2009. The LCLS includes several ultrafast science instruments: the X-Ray Pump Probe (XPP), X-Ray Correlation Spectroscopy (XCS), and Coherent X-ray Imaging (CXI); ARRA funding accelerated these accomplishments.
- The Transmission Electron Aberration-Corrected Microscope (TEAM) transitioned to a User Facility. TEAM's successful conclusion is a historic achievement for electron microscopy.
- Groundbreaking was held in June 2009 for the National Synchrotron Light Source-II. The Advanced Light Source User Support Building is under construction.
- New hires at BES include an American Association for the Advancement of Science (AAAS) research fellow and user-facility overseers.

The BES FY10 appropriations Conference Report said that "The conference agreement provides $1,636,500,000 for Basic Energy Sciences. Within these funds, the conference agreement provides $22,000,000 for the Experimental Program to Stimulate Competitive Research (EPSCoR), and directs the limit of one Implementation Grant per EPSCOR state be removed and the cap on the maximum allowable award be increased to $2,500,000. The conference agreement provides no funds for an Energy Innovation Hub within the Office of Science. Further, the conferees include funding as requested for the Spallation Neutron Source and the High Flux Isotope Reactor. " In this budget appropriation, are $100 million for the EFRCs (no change from FY09); a 3% increase for grand-challenge science, accelerator, and detector research; $22 million for EPSCoR; and a 3% increase for scientific-user-facility operations. Construction and instrumentation are also being funded.

Dr. Kung answered questions posed by the panel.

Question: Will BES interface EERE on the EFRCs?
Answer: Yes, and with industry too.

Question: While three hubs are funded in the FY 10 budget, none is funded from the BES budget?
Answer: That's correct. Funding will come from the EERE budget in FY10, and each hub will be funded at $20 million with infrastructure funding coming from the ARRA.

Question: Will flexibility in management be encouraged?
Answer: Flexibility is encouraged but BES will actively monitor changes. The teams will document changes, but BES will not limit changes. Rather, it will look at results. A report has to be made to Congress on how that is to be done.

Question: Will there be more than one fourth-generation light source?
Answer: Yes. It's a class.

Question: Will the fuels-from-sunlight hub be managed by SC even though the money comes from EERE?
Answer: Yes. SC had the lead, but SC and EERE are working together to direct the program, just as SC is working with NE on the nuclear-power hub.

A break was declared at 10:15 a.m. The meeting resumed at 10:34 a.m.

Harold Shapiro and **Peter Blair**[3] were asked to discuss the report *America's Energy Future: Technology Opportunities, Risks, and Tradeoffs*[4]. The report was issued by the National Academies in September 2009. It presents energy-technology options that could be implemented at scale for the next few decades. Given the size and complexity of the sector, there are roadblocks everywhere. There were 63 committee and panel members. The project was sponsored by DOE, the Keck and Kavli foundations, Dow Chemical, General Electric, Intel, General Motors, BP (British Petroleum), and the National Academies.

The basic concerns were:

- environmental issues emanating from the burning of fossil fuels with inadequate accounting for the serious externalities involved;
- national-security issues emanating from the falling production of petroleum, the dependence on fragile supply chains, the vulnerability of the electrical grid and the transportation sector, the infrastructure getting older and more vulnerable, and nuclear safety and proliferation; and
- economic competitiveness in the face of volatile prices for energy supplies and uncertainties that surround the various supply chains.

Initial conditions matter a lot. What struck the panel was that the United States is a large and not very efficient user of energy. Increasing energy efficiency (doing exactly what is being done now but with less energy) pays dividends. Eighty-five percent of U.S. energy is created through the burning of fossil fuels with traditional technologies. Much of the U.S. energy sector's physical assets are old and deteriorating, including. The transportation sector is almost fully dependent on petroleum.

The AEF Committee's overall conclusion is that the only way to meet the concerns identified given our initial conditions is to embark on a sustained effort to transform the manner in which we produce and consume energy. There is no silver bullet. The AEF Committee carefully considered some of the critical technological options (including their costs and limitations). The AEF Committee looked at energy efficiency; alternative transportation fuels; renewable electric power generation; natural gas and advanced coal-fired power generation and CO_2 capture and storage; nuclear power; and electric power

[3] The full presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0924
[4] The full report can be found at: http://www.nap.edu/catalog/12450.html

transmission, distribution, control, and storage. It did not consider conservation (changes in lifestyle); improvements in exploration, extraction, and transportation of primary energy sources; or a fuller assessment of worldwide primary energy resources.

The panel's recommendations are presented in eight "findings":

1. With sustained effort, there is a potential for transformational change. The United States could obtain substantial energy-efficiency improvements, new sources of energy, and reductions in greenhouse gas emissions through the accelerated deployment of existing and emerging energy-supply and end-use technologies.
2. The deployment of existing energy-efficiency technologies is the nearest-term and lowest-cost option for moderating our nation's demand for energy, especially over the next decade.
3. The United States has many promising options for obtaining new supplies of electricity and changing its supply mix during the next two to three decades, especially if carbon capture and storage (CCS) and evolutionary nuclear technologies can by deployed at required scales. However, the deployment of these new supply technologies is very likely to result in higher consumer prices for electricity.
4. Expansion and modernization of the nation's electrical transmission and distribution systems (the power grid) are urgently needed.
5. Petroleum will continue to be an indispensable transportation fuel through at least 2035. Alternative liquid fuels make a contribution, but do not change our dependence on petroleum.
6. Substantial reductions in greenhouse-gas emissions from the electricity sector are achievable over the next two to three decades through a portfolio approach involving the widespread deployment of energy efficiency; renewable energy; coal, natural gas, and biomass with CCS; and nuclear technologies.
7. To enable accelerated deployments of new energy technologies starting around 2020, and to ensure that innovative ideas continue to be explored, the public and private sectors will need to perform extensive research, development, and demonstration over the next decade.
8. A number of barriers could delay or even prevent the accelerated deployment of the energy-supply and end-use technologies described in the report. Policy and regulatory actions, as well as other incentives, will be required to overcome these barriers.

Following the presentation, the BESAC members posed a number of questions:

Question: Why was conservation left out?
Answer: Efficiency is in building codes, light-bulb technology, etc. Conservation is about behavior, and the Committee did not know how to get people to change their lifestyles.

Question: There seems to be no mention of hydrogen?
Answer: Hydrogen may be a big part of energy use in 50 years.

Question: When there is a transformational technology, it changes the face of what is going on (e.g., the Internet). Had the NAS Committee given any thought regarding how to anticipate or to move swiftly with transformational technologies?
Answer: There will be a transformational technology sometime but it's not clear when. An insurance policy was needed. Society needs to get on with what it has in order to get to the time when breakthroughs occur.

Linda Blevins[5] was asked to discuss the Early Career Research Program (ECRP) and the evolution of the DOE data systems. In response to several studies, the ECRP supports outstanding scientists early in their careers and stimulates research careers in the disciplines supported by the Office of Science. Design and development of the program was done by program managers from across SC. The program identifies principal investigators within 10 years of receiving a PhD who are either untenured academic assistant professors on the tenure track, or full-time DOE national-laboratory employees. About 65 awards are expected in FY10 with $85 million in Recovery Act funds. Future annual competitions will be supported through regular research appropriations.

University grants are at least $150,000 per year for 5 years and cover summer salary and expenses. National-laboratory awards are at least $500,000 per year for 5 years and cover full annual salary and expenses. Announcements were posted July 2, 2009. About 2200 letters of intent arrived by August 3. About 1750 full proposals arrived by September 1. BES is reviewing about 850 proposals, and announcements are expected by February 1, 2010. Research grants will be competitively awarded based on peer review. Review and award management will take place in the six science programs. Eligibility criteria, review criteria, and program rules are common across SC.

In May 2008, the SC Office of Business Management initiated a project to develop requirements for a grants-management data system. A team of six program managers, one from each SC program, with input from support staff members from across SC, developed the requirements. The Portfolio Analysis and Management System (PAMS) comprises a core database with flexibility to add data manipulation modules. It exchanges data with existing systems, allowing input from inside DOE as well as outside. Examples of input include reviews, revised budgets, progress reports, people profiles, workforce forms, etc. It amasses a proposal record that includes the electronic proposal, correspondence, reviews and review information, documentation of the decision, post-award management documents, and various metadata. This record is the people record, which covers information about reviewers and principal investigators with their contact information, optional demographics, keywords, and proposal/review history.

The additional features that PAMS will have are time and date stamping, tracking, built-in notifications and reminders; data aggregation, sorting, and calculations; easy access for program managers to the portfolio; search ability on all data fields; privacy controls; and facilitation of a public abstracts database. The data challenge for PAMS is that SC employs about 150 federal program managers.

[5] Dr. Blevins' presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

At any given time, SC manages about 3000 financial-assistance awards and more than 1000 national-laboratory awards. SC annually receives about 2500 new, renewal, and supplemental financial-assistance applications, with each proposal receiving three to five reviews. So SC collects more than 10,000 reviews annually. As a result, SC annually supports about 25,000 people (PhDs, graduate students, undergraduate students, engineers, and technicians). The timing for implementing PAMS is not certain, but SC is committed to this and is working hard toward this goal.

Following Dr. Blevins presentation, the committee asked several questions:

Question: Why are home addresses collected?
Answer: The Graduate Fellowship Program is open to people who do not have an institutional address, so home addresses had to be collected.

Question: Would there be a call every year?
Answer: Yes. Universities are being forward funded for 4 years and national laboratories for 5 years out of the ARRA funds, and there will be annual competitions.

Question: This year the Fellowship Program was an SC project. Will it always be so?
Answer: WE expect it would always be an SC project with allocations to the different SC offices.

Question: Out of the 65 awards, how many would be national-laboratory awards and how many would be university awards?
Answer: 45 university and 20 national-laboratory awards will be made.

Question: How fine-grained would the data sets be and would we be able to see patterns?
Answer: In principle, high granularity could be done. It would allow analysis of budgets. One wants as much granularity as possible to show success rates, numbers of proposals submitted, etc. Modules will be added later to pull such statistics out.

Question: What was the expected proposal submittal rate?
Answer: An estimate was made. The Office expected 1500 applications and got 3000 letters of intent. The revised proposal rate was then publicized on the web. This was an ARRA program. It was a tremendous response, which required a lot of reviewers.

A break for lunch was declared at 12:02 p.m.

Thursday, November 5, 2009
Afternoon Session

The meeting was called back into session at 1:30 p.m. **William Barletta** and **John Corlett** were asked to report on the BES workshop on *Accelerator Physics for Light Sources*[6] that looked at machine limitations and possibilities. The purpose of the

[6] The presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

workshop was to provide a technical basis for BES investment in accelerator R&D. Meeting for 2 $^{1}/_{2}$ days, the 50 participants discussed electron lasers, energy-recovery linacs, and ultimate storage rings. The workshop included plenary presentations, and working-group meetings, including one session on instrumentation and detectors. The papers were submitted as a set to *Nuclear Instruments and Methods*.

With the LCLS, free-electron lasers (FELs) are now proven from the infrared (IR) to the hard X-ray range. Directions for FEL developments are to increase the average flux and brightness; to enhance temporal coherence; to control pulse duration and pulse energy; and to extend the photon energy range.

The Freie-Elektronen-LASer (FLASH) in Hamburg, which operates in the ultraviolet, and the LCLS have pushed up the peak brightness by 10 orders of magnitude. Future directions are an increase in brightness via superconducting rf systems and high-repetition-rate injectors. Bandwidth and pulse length will be pushed down by transform-limit shorter pulses and by seeding to get very low bandwidths. The repetition rate will be increased, and the pulse-duration gate and photons per pulse will be pushed down.

R&D priorities include robust photocathodes with high-efficiency, low-intrinsic-emittance, and high-current; injectors with high-brightness, flexibility to incorporate beam manipulations, and high-repetition-rate (tens of kilohertz to megahertz and beyond); laser manipulations and seeding techniques; and high-average-power laser systems (dependent on developments in photocathodes and seeding techniques). At the workshop, several of these areas came up as cross-cutting issues.

R&D is needed in RF structures and power, undulators, diagnostics, simulation tools, etc. There are test beds at several laboratories, including BNL and the LCLS in the U.S., and several in Europe. A low-repetition-rate facility could test coherent emission from laser-manipulation, seeding, self-seeding, oscillator, and short-bunch techniques. A high-repetition-rate facility could test high-brightness-photocathode, gun, and injector designs.

In terms of timescales, a 1-kHz soft X-ray is ready to be built today, and a 10- to 100-kHz soft X-ray facility could be ready to be built within 3 to 5 years. Ultra-short bunches with a coherence length of about 1 fs are ready today. Laser manipulations for soft X-rays of greater than 10 kHz will be achievable within 3 to 5 years. And self-seeding and oscillators for hard X-rays will be available in 5 to 10 years.

To extend the photon energy to tens of kilo-electron volts, undulator technology could have a big payoff in 3 years; high-frequency, high-gradient RF structures would take 3 to 5 years; and novel acceleration methods will be available further out (more than 10 years).

The concept of the Energy-Recovery Linac (ERL) X-ray Source was envisioned as a high-brightness, high-average-current, 10-MeV injector; a merger; a multi-GeV superconducting linac; a multi-GeV output beam; a turnaround arc with a lattice of undulators; and a multi-GeV return beam.

Today in ERLs, there are demonstrated:

- a 9-mA continuous-wave (CW) two-pass at 30 MeV facility at the Budker Institute for Nuclear Physics (BINP);
- a 9-mA CW at 150 MeV facility at the Jefferson Laboratory (JLab) FEL, and
- a 70-µA CW at 1 GeV facility at JLab's Continuous Electron Beam Accelerator Facility (CEBAF).

In the hard X-ray range, the goal is for hundreds of milliamps with a beam emittance that is about 10 to 100 times smaller than what has been demonstrated, multi-GeV, and a 100-MW beam power.

In ERL development, the diffraction limit for hard X-rays should be approached with a high-brightness, high-energy beam with a small energy spread. For high average flux and brightness, again what is needed are a high-brightness, high-repetition-rate photo-injector; optimized CW superconducting rf systems; energy-recovery physics; and a high beam power. One can reduce the bandwidth by maintaining a small energy spread in the beam from the injector and can reduce the pulse duration with a dedicated high-brightness injector. In terms of average brightness, ERL allows a several-orders-of-magnitude increase. Bandwidth can be pushed down with third-generation storage rings and small energy spread injectors, which allows one to use the undulators to the full extent. The repetition rate will be pushed down by short pulses and bunch trains.

For ERL physics and technology, the R&D priorities are photocathodes, injectors, the drive laser, and recirculation and energy recovery. A lot of power has to be handled, so rf structures and power have to be studied. ERL research, development, and demonstration (RD&D) needs include undulators, diagnostics, and X-ray optics.

Testbeds exist at the CEBAF, JLab FEL, Cornell R&D ERL, and BNL R&D ERL. An injector test facility for ERLs is needed to test photocathode, gun, and injector designs; drive laser; and beam merger with a very high repetition-rate, recirculation, and energy recovery. The timescales for these developments are a high brightness injector in 3 to 5 years and an ERL test facility demonstrating critical hardware and physics in about 10 years.

Ultimate storage rings are a well-developed and well-understood technology with a high average brightness and flux, a high current, a high repetition rate, high stability, easy and rapid tunability, and high-reliability service for many users with multiple requirements. The goal for ultimate storage rings is to approach the diffraction limit in the electron beams for hard X-rays, and high average flux and brightness are needed, requiring a several-GeV beam power, a few-kilometer circumference, frequent injection, a couple of seeds, matching electron and photon space orientation, and partial lasing at longer wavelengths. Future storage rings will allow ERLs to increase the average brightness.

R&D needed for ultimate rings include improved code development and simulation and dynamic aperture. Injection systems with a ring with a larger dynamic aperture allow for accumulation, and a ring with a smaller dynamic aperture requires on-axis injection.

R&D on bunch manipulations, instrumentation and diagnostics, short-period undulators, rf cavities and power, and detectors is also needed.

Almost all the required accelerator physics and technologies to realize an ultimate storage ring are in hand. What is needed is to complete an integrated design that optimizes the performance. The design will be mature in about 5 years.

Other sources were largely laser-based ones, such as lasers generating extreme-ultraviolet radiation for high harmonic generation (HHG) that would extend ultrafast pulses into the extreme ultraviolet and act as seed for soft X-ray (SXR) FELs. Lasers can be used as alternates to "conventional" technologies. Laser-plasma accelerators (LPAs) today are compact electron sources with extremely high fields. Electron beams have been demonstrated with 10 pC, <50 fs, a few-percent energy spread, less than 1 mrad of divergence, and about 1 GeV of energy. Laser-driven vacuum structures are less mature; they are all-optical accelerators and undulators with an up to 1-GVm^{-1} accelerating gradient. There are also inverse Compton sources. These are potentially of low cost.

Other sources need R&D in laser-plasma accelerators (tailored plasma channels, injection and acceleration schemes, diagnostics, 3-D simulation codes, and short-period undulators), laser-driven vacuum structures (basic proof-of-principle experiments for key concepts and sub-femtosecond synchronization, materials damage, charging of structures, and diagnostics for beams), and inverse Compton sources (high-brightness, high-beam power injectors; laser build-up cavity, and integration of the laser and the CW superconducting-rf accelerator).

RD&D in high-power lasers (about 100 W in the IR) will enable unique HHG-based extreme-ultraviolet sources that could be used as a stand-alone source or for FEL seeding, be a source for testing equipment and preparation for measurements at FELs, be essential for laser-plasma acceleration and laser-driven vacuum structures, and as experimental lasers to match the FEL repetition rate. Such lasers might be achieved with diode-pumped amplifier performance, ceramics, new crystals, fiber multiplexing and optical-cooling and damage issues. Laser technology is rapidly evolving, and HHG and LPA-based sources are rapidly maturing.

The enabling instrumentation and technology group identified insertion devices and ultrafast instrumentation, cathodes, photon detectors, insertion devices, and high-power lasers as being needed.

The Committee had several questions and comments following the presentation.

Question: Was there anything about high-risk/high-payoff options?
Answer: There is some of that "other sources," where there has to be great improvements in, say, beam quality.

Comment: Many ideas will need much more beam time. The number of users a facility can serve will be an important parameter.

Question: 90% of what was presented can be done in 3 to 5 years. What resources would be needed?
Answer: The programs need to be fully funded. The workshop did not look at costs, but they would run in the tens of millions of dollars per year.

Question: Is the staffing adequate?
Answer: The resources to pursue a number of these paths are in hand. It is mostly a matter of what direction science pushes in. The testbeds would tell what the "real machine" could do and would look like. For the next 5 years, the only X-ray femtosecond laser will be the LCLS. He noted that an executive summary has been turned in to Harriet Kung and Pedro Montano. It will be available to the public in about a month.

Mary Galvin[7] was asked to report on post combustion carbon-capture. In presenting the background and challenges for capturing carbon dioxide from coal-fired electric power generating facilities, Dr. Galvin noted the three categories of CO2 capture: post-combustion, pre-combustion, and oxy-combustion. Challenges for post-combustion capture include low CO2 concentration in the flue gas, and the high energy penalty for regenerating the capture medium. Pre-combustion capture generally would require building new plants to include coal gasification units. And both pre-combustion processes and oxy-combustion processes would require expensive air separation units to produce oxygen.

Dr. Galvin noted two DOE sponsored workshops on carbon capture: the first led by the Office of Fossil Energy (FE), and held at the University of Maryland October 5-6, 2009; and the second to be led by the Office of Science in February or early March, 2010.

The FE-led workshop was *Carbon Capture 2020*. Its goals were:

- to communicate the status so that the research community understands the challenge, and
- to produce a roadmap for a coordinated effort that will impact carbon capture by 2020.

The workshop had a welcome session; background talks; breakout sessions on solid sorbents, liquid absorbents and solvents, membrane concepts, cross-cutting issues, and chemical and biological analogues; and poster sessions.

The Office of Science-led carbon-capture workshop will focus on carbon capture beyond 2020. Fundamental science needs to advance existing approaches more rapidly, and new approaches and materials that would require significantly less parasitic energy to separate the CO_2 need to be identified. The workshop will be run like a Basic Research Needs Workshop, and will include plenary talks on technical and scientific challenges, breakout panels focused on development of priority research directions, and a crosscutting panel focused on identification of grand challenge science themes. Paul Alivisatos and Michelle Buchanan will chair this workshop in the D.C. area.

[7] Dr. Galvin's presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

The Committee had several questions and comments following the presentation.

Question: What were the costs were of the best-available technologies and where could those costs could be cut?
Answer: Estimates suggest 20% increase for all technologies. For post-combustion carbon capture, the stripping takes up 35% of the energy, and the rest is in compression. This process adds 30 to 50% to the electricity cost.

Question: Where would the CO_2 be put?
Answer: It will be stored underground, for example in saline aquifers. In Australia, they have stored CO_2 underground for 10 years without a leak. The United States has a lot of such aquifers. That is not true elsewhere. The cost estimates include these sequestration costs.

The Committee noted the risk of a seismic event could potentially release gigatons of CO_2 and asphyxiate millions of people.

A break was declared at 3:01 p.m. The meeting was called back into session at 3:28p.m.

Dr Hemminger initiated a discussion of the BESAC Energy Roadblock Workshop. The charge letter said, "I would now like BESAC to pursue a follow-on study to those of the past seven years that links basic research with more applied problems in energy technologies. This study should tie together the ten BES reports on Basic Research Needs for energy technologies. This new study should be regarded as the companion study to the grand challenges report, but with a focus on the basic science drivers that will be essential to the more applied issues of energy science."

The letter recommended:

1. Summarizing the science themes that emerged from the BESAC report *Basic Research Needs for a Secure Energy Future* and the follow-on *BES Basic Research Needs* topical reports with an emphasis on the needs of more applied energy technologies while identifying grand-challenge science drivers that are likely to have an impact in the energy arena in the near term.
2. Identifying how the suite of BES-supported and -managed scientific user facilities can impact basic and applied research for energy.
3. Identifying major impediments to successful achievement and implementation of transformative energy technologies, including potential deficits in human capital and workforce development, and possible solutions to these problems.

This activity should produce two reports, a short one like the *New Era* report and a more technical report for the scientific community. The *Grand Challenge* and *New Era* reports had a significant impact and led to the next report, *Science for Energy Technology*. A BESAC subcommittee is being put together to conduct a workshop. George Crabtree has agreed to cochair it with Alex Malozemoff. The study will look at how BES should be interacting with the applied technology offices of DOE and with industry. There will be a strong industrial component in this study group. There will also be a workshop in late January 2010 at the Rockville Hilton Hotel. The workshop will identify industry needs to implement transformative energy technology and to identify science solutions to fill industry needs.

Dr. Hemminger then opened the floor for discussion about the workshop. The Committee wanted more background on the intent of the charge. Dr. Hemminger indicated that that there is a fundamental interest in having BES's science address national needs, such as improving industrial competitiveness. There was considerable discussion of the role and accomplishments of industrial laboratories such as Bell Labs and General Electric (GE) research labs, and technology transfer. It was noted that both labs are gone from the industrial landscape. They are no longer creating technology and passing it through to the market. Many industries thought they could fill the innovation pipeline at universities. But there is no one pipeline, and many industries went overseas for cheap science labor. These strategies did not always work out. The upcoming workshop should examine these questions holistically.

Dr. Hemminger suggested that BESAC advises SC what BES should do. At the end of the workshop report, BESAC's thoughts about programs for SC and BES should be given. He also noted that there would be a shorter, 10 to 14 page report.

With regard to technology transfer, the Committee noted that industry does not need to be taught how to do technology transfer. Policy changes such as R&D tax credits, patent reform, etc. are needed. The outcome of the workshop should be to help grow the base of BES to serve the needs of society. The Committee was unclear whether this report is to be focused on the near-term, such as the question, "What does industry need now?"

Dr. Hemminger pointed out that many of the Basic Research Needs reports (BRNs) had science issues that could connect science with industry. The BRNs that have been done could be mined, for example, for cost-cutting issues. Also, this report is to point to what *else* BES should be doing. There is a need to educate the academic scientific community. They do not know what the problems are (e.g., why a lithium-ion battery fails).

The Committee expressed concern that the report be specific enough to be helpful to university researchers. In prior reports, there are lists of basic science needs. However, they often are too general to be of use.

Dr. Hemminger opened the floor to public comment. There was none.
The meeting was adjourned for the day at 4:52 p.m.

Friday, November 6, 2009
Morning Session

Dr. Hemminger called the meeting to order at 9:00 a.m. He announced that BESAC had been asked to conduct a committee of visitors (COV) for the Office of Workforce

Development for Teachers and Scientists (WDTS). **William Valdez**, the Director of WDTS, was asked to describe the Office and its programs[8].

The mission of WDTS is to help ensure that DOE and the nation have a sustained pipeline of highly trained science, technology, engineering and mathematics (STEM) workers. Priorities are:

- to contribute to the development of STEM K–16 educators;
- to provide mentored research experiences to undergraduate students and faculty;
- to increase opportunities for under-represented students and faculty; and
- to provide graduate fellowships.

The core activities of WDTS are conducted at national laboratories and in partnerships with universities. This allows participants access to cutting-edge research and content, unique facilities and immense infrastructure, and world-class mentors. WDTS takes this pipeline approach to programs for high school and middle school teachers, undergraduate internship programs, and graduate programs.

In student programs, WDTS works with the DOE national laboratories to provide mentor-intensive research experiences to students and faculty and it sponsors competitions designed to encourage and inspire students to participate in the STEM arena.

In educator programs, WDTS is working to improve the ability of educators at the K-16 level to teach STEM content and methods is a key to improving student achievement and developing a long-term STEM pipeline through DOE Academies Creating Teacher Scientists (ACTS), Albert Einstein Distinguished Educator Fellowship, and Faculty and Student Teams (FaST).

Most important is to align the WTDS program with the needs of SC research programs. The disciplines of SC need to be supported. Discussions are held with the offices of SC to assure that the areas supported are the ones of interest to the offices.

WDTS participates in partnerships with other agencies and organizations to leverage its assets. Funding for the Office was

- $6 million in FY07,
- $8 million in FY08,
- $16 million in FY09, and
- $21 million plus $5 million in ARRA funding in FY10.

In the leaner years, an emphasis is put on partnerships. Under a National Science Foundation (NSF) memorandum of understanding (MOU), the NSF provides funding for undergraduate research internships and FaST Teams, and there is emerging cooperation on minority-serving-institution STEM Training Programs. The California State

[8] Mr. Valdez's presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0924

University System participates in the Science Teacher and Researcher (STAR) program with NSF Noyce and NASA Centers.

The DOE National Science Bowl gets 5000 volunteers from industry and academia. DOE funds 6 Einstein Fellowships, and NSF, National Institutes of Health (NIH), NASA, National Oceanic and Atmospheric Administration (NOAA), etc. fund 13. The National Science and Technology Council (NSTC) Education Subcommittee is very useful in coordinating and info sharing of best practices and partnerships.

Planning in FY10 includes interagency coordination through the NSTC Education Subcommittee. A COV review will be conducted in May 2010. The annual evaluation cycle will include laboratory self-appraisals, participant surveys, and a new workforce study/analysis. An updated Strategic Plan will be released in early 2010. Finally, there is a potential National Academy of Engineering workshop and study of engineering education in the United States.

WDTS's benefits include giving students opportunities to make an informed choice about pursuing a STEM career; giving students and faculty with an aptitude and desire the opportunity to pursue STEM careers and education; and providing students and faculty with a pathway to STEM careers at DOE, its National Laboratories, and other institutions.

A review of the funding history of the WTDS program invites an air of caution. In 1990, the Secretary decided he wanted a significant education program at DOE. The 1991 Science Education Act increased DOE funding for science education to $60 million per year. However, 1996, the Congress questioned DOE's involvement in education, and the program was zeroed out because it was not aligned with the DOE mission. In 1999, a rebuilding effort started at about $3 million, trying to stay true to the two core principles. Today, funding is approaching $20 million per year.

The Committee had several questions and comments following Mr. Valdez's presentation.

It was suggested that members of the scientific community need to work hard to make sure that such a scenario is not repeated.

Question: What is the status was of the Graduate Fellowship Program?
Answer: The Graduate Fellowship opened on Sept. 30, 2009. It closes on Nov. 30. The Office is overwhelmed with applications. The response has been comparable to that of the NSF's graduate fellowship program.

Question: Will there be an annual call for fellowships?
Answer: Yes.

Question: Will the budget will be the same?

Answer: The program will be able to support 160 to 180 in the 2010–2011 academic years. It is hoped to increase the number to 300 or 400 in the out years.

Question: Does WDTS put support into curriculum development?
Answer: That is the turf of NSF and the Department of Education. On the other hand, some of the teacher interns involved in WDTS programs have developed content that is being brought up on the website of DOE’s Office of Scientific and Technical Information (OSTI). WDTS is working with the National Geographic, the Discovery Channel, NASA, NSF, etc. to put their content up on that website, also. It is also working on a cyberlearning program to get this content into classrooms.

Question: What is the number of graduate research fellowships?
Answer: The number is 1000 per year; 3000 per cohort.

Nora Berrah was asked to share some of the early progress at the LCLS. The LCLS started lasing in April 2009. The first light in the atomic, molecular, and optical science (AMO) instrument was in August 2009. User operation during LCLS commissioning started October 1, 2009. Beam time was allocated by competition. This machine offers the possibility of a leap forward in the understanding and control of the interaction of matter with ultra-fast and ultra-intense electromagnetic radiation at the molecular and atomic levels. This research could contribute to three BES grand challenges:

- How does one control material processes at the level of electrons?
- How do remarkable properties of matter emerge from complex correlations of the atomic or electronic constituents; and
- How can one control these properties; and how does one characterize and control matter under extreme conditions?

An experiment conducted at the FLASH facility was turning solid aluminum transparent by intense soft X-ray photo-ionization. Saturable absorption (SA, the decrease in the absorption of light with increasing intensity) of a metal in the soft X-ray regime led to transparency to vacuum ultraviolet at 92 eV. SA creates highly uniform, warm, dense conditions, a regime of great interest in high-pressure science. It also leads to the storage of 100 eV per atom, evolving to a warm, dense state.

Study of finite quantum systems, atoms, molecules, and clusters under extreme conditions with the LCLS is fundamental to many scientific fields. Direct applications include single-shot biomolecule imaging. It is expected that AMO research will ultimately provide the means to minimize damage effects using doped clusters.

The LCLS has six hutches, one of which is for the AMO instrument. The goals of the first AMO experiments were:

1. To understand the nature of high-intensity X-ray photo-absorption processes, nonlinear processes, and multiphoton, multi-electron core ionization in atoms, molecules, and clusters.

2. To explore and understand the formation dynamics of multiple-core-hole states in atoms, molecules, and clusters and the mechanisms for their subsequent fragmentation dynamics.
3. To exploit laser-induced molecular alignment to control the molecular frame direction of core-electron removal and to control the resulting fragmentation dynamics.

The properties of interest result from multiphoton ionization, two electrons absorbing two photons or one electron absorbing two photons. Time-of-flight (TOF) spectrometers at five different angles were used to detect different types of electrons. The optical laser and LCLS synchronization effort was made in collaboration with other national laboratories.

Four experiments have been conducted. Two were to understand the nature of the high-intensity X-ray photo-absorption process and multiphoton multi-electron core ionization in neon. The nature of multiphoton X-ray absorption is not clear. With a short pulse, one can have absorption of two photons before the Auger state occurs, a new form of ionization and a new form of matter.

The process is energy dependent. At 800 eV, which is less than the neon 1s binding energy, high Q is produced by valence ionization only, and six photons are absorbed sequentially. At 990 eV, which is less than the neon $1s^2$ binding energy, PAPA (photon absorption, Auger state, photon absorption, Auger state) dominates (with odd-even alteration), and seven photons have been observed to be absorbed sequentially. In this first experiment, the double absorption was obtained, as indicated by the detection of the PPA signature.

The third experiment was designed to explore and understand the formation dynamics of multiple-core-hole states in molecules and the mechanisms for their subsequent fragmentation and relaxation dynamics. The molecules of interest were N_2, CO, H_2S, and SF_6. Normally, one sees a peak in counts and then Auger decay. But several absorption mechanisms were being looked for, so the intensity was varied to see the intensity dependency of the different absorption mechanisms.

Indeed, the nitrogen molecule was stripped of seven electrons. The short pulse suppressed Auger dynamics. It would be a higher damage threshold for biomolecules; they are more transparent in the X-ray regime. Diffraction-pattern images will be able to be obtained for biological samples. The nitrogen electron spectra were investigated as a function of pulse length, and the formation of a double four-four ionization of N_2 was found.

In carbon monoxide ionization, the ion-mass spectrum showed the entire multi-photon absorption. To see if there were two-photon absorptions, one had to go below the K shell in sulfur molecules (H_2S and SF_6). With SF_6, one gets ionization of the fluorine, also; therefore, the sulfur and fluorine get ionized up to 14^+.

The fourth experiment was the first X-ray/optical alignment and pump probe experiment to commission the laser–X-ray system. Temporal and spatial overlap allowed the N^+ and N_2^{++} signals to be cumulated, and moving the laser around allowed optimizing the conditions for observing the N_2^{++} peak.

Future experiments will look at the conversion of light to other forms of energy. Conical intersections are not understood and could be probed in a variety of molecules under a variety of conditions to study electrodynamics and charge transport. Hole-migration dynamics may also be studied, and few-femtosecond and attosecond electron dynamics may be observed along with the structure determination of big clusters to examine radiation damage and Coulomb explosions.

There is the possibility of shorter pulses at the LCLS: In the few-femtosecond mode, the electron bunch charge is reduced from 250 pC to 20 pC, resulting in a shorter electron bunch. According to simulations, 2-fs pulses are possible. In the attosecond mode, even shorter pulses are possible with the echo technique, which employs co-propagation of the laser and electron bunch in a wiggler to produce micro-bunching.

In terms of the user experience at the LCLS, the management is very concerned with safety, and the accelerator physicists are very interested in the experimental details so they can provide the desired beam properties.

The Committee had several questions and comments following Dr. Berrah's presentation.

Question: What are the lifetimes of the multiply-ionized species?
Answer: They vary from 3 to 7 fs.

Question: How were the angles chosen and can one do coincidence measurements?
Answer: What was to be measured was the angular distribution of the photoelectrons and the Auger electrons. The photoelectrons move around with their energy. The Auger electrons always are in the same place. So one photoelectron detector is at 0°, another is at a magic angle (which is parallel to the electron dipole and the intersection of the dipole lobes), and two detectors are in the nondipole plane. Coincidences are not done now, but there is hope to get to them in the second or third cycle.

Question: Were the lifetimes of the ionizations a surprise to the researchers and the machine people?
Answer: Yes. The machine people were able to compress the bunches and give shorter pulses.

Question: Can clusters of biomolecules be able to be probed without damage?
Answer: That is in the future. A biomolecule will be looked at at the end of November. Other scientific disciplines want to use this AMO machine. It will be difficult to get beam time.

Dr. Hemminger opened the floor to discussion of the proposed roadblock workshop. A list of commercial successes that have come out of BES funded research was distributed[9]. The charge[10] was projected on the screen, and Dr. Hemminger said that a lot of what was being talked about was in the BRNs.

The Committee grappled with various terms of reference in the charge letter, and seemed concerned about the phrases “near term” and “more applied energy technologies.” The extent of industry involvement was discussed, with the recommendation that the Committee should be inclusive in its response to the charge. Dr. Hemminger reassured the Committee that the intent was not to refocus BES into a short term job shop. He asked the Committee members to send e-mails to him if they had any additional thoughts. Weekly teleconferences should be set up with the workshop co-chairs.

The workshop will be will be held on January 19–21, 2010, at the Rockville Hilton Hotel and Conference Center. The next BESAC meeting will be March 2–3 at the Bethesda North Marriott.

Dr. Hemminger opened the floor to new business. There was none. He then opened the floor to public comment. There being none, the meeting was adjourned at 11:17 a.m.

Respectfully submitted,
Frederick M. O’Hara, Jr.
Recording Secretary
Dec. 2, 2009
(Edited 12/29/09 MIS)

[9] INSERT THE LIST HERE
[10] The charge letter, “Companion Study on Grand Challenges for Applied Issues of Energy Science” can be found at: http://www.er.doe.gov/bes/besac/reports.html