Minutes of the
Basic Energy Sciences Advisory Committee Meeting
March 2–3, 2010
Bethesda North Marriott Hotel and Conference Center
Rockville, Maryland

BESAC members present:

Simon Bare
Nora Berrah
Sylvia Ceyer
Peter Cummings
Mostafa El-Sayed
George Flynn
Bruce Gates
Laura Greene
John Hemminger, Chairman
Bruce Kay
Kate Kirby
William McCurdy, Jr.
John Richards
John Spence
Kathleen Taylor
John Tranquada

BESAC members absent:

Sue Clark
Frank DiSalvo
Sharon Hammes-Schiffer
Daniel Morse
Martin Moskovits
Douglas Tobias

Also participating:

William Brinkman, Director, Office of Science, USDOE
Altaf Carim, Program Manager, Scientific User Facilities Division, Office of Basic Energy Sciences, USDOE
Julie Carruthers, Office of the Deputy Director for Science Programs, Office of Science, USDOE
George Crabtree, Associate Director, Materials Science Division, Argonne National Laboratory
Patricia Dehmer, Deputy Director for Science Programs, Office of Science, USDOE
Linda Horton, Director, Materials Science and Engineering Division, Office of Basic Energy Sciences, USDOE
Alan Hurd, Director, Lujan Neutron Scattering Center, Los Alamos National Laboratory
Harriet Kung, Associate Director of Science for Basic Energy Sciences, USDOE
Alex Malozemoff, Chief Technical Officer, American Superconductor Corporation
Celia Merzbacher, Vice-President for Innovative Partnerships, Semiconductor Research Corporation
David Miller, Director, Science and Engineering Division, Idaho National Laboratory
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
Rachel Smith, Oak Ridge Institute for Science and Education

About 100 others were in attendance in the course of the two-day meeting.

Tuesday, March 2, 2010
Morning Session

Before the meeting, Wayne Gordon of the DOE Office of the General Counsel briefed the Committee members on ethics, and Rachel Smith made convenience and safety announcements.

Chairman **John Hemminger** called the meeting to order at 8:34 a.m. and had the members introduce themselves. He introduced **William Brinkman**[1] to present the Office of Science (SC) FY 2011 budget request to Congress.

The request for Basic Energy Sciences (BES) goes up 12%; for Advanced Scientific Computing Research (ASCR), 8%; for Biological and Environmental Research (BER), 4%; and for Nuclear Physics (NP), 5%.

SC supports 27,000 Ph.D.s, graduate students, undergraduates, engineers, and technicians and 26,000 users of world-leading, open-access facilities. It provides support to 300 leading academic institutions and all 17 DOE laboratories. Light sources constitute about one-third of its budget.

The FY11 budget includes:

- a new hub;
- enhanced activities in climate science and modeling (including the effects of clouds and aerosols);
- $66 million spread among individual investigators, small groups, and Energy Frontier Research Centers (EFRCs);
- leadership computing facilities; and
- multiscale modeling of combustion and advanced engine systems;
- full funding of the scientific user facilities; and
- expansion of the education and workforce development programs;
- funding in all of the SC research programs for the SC Graduate Fellowship Program and the SC Early Career Research Program (ECRP).

DOE has three hubs this year (FY 2010): Fuels from Sunlight, Energy-Efficient Building System Design, and Modeling and Simulation of Advanced Nuclear Systems. Proposals for the Fuels from Sunlight hub are due in March. The new proposed (FY 2011) hub is the Batteries and Energy Storage Energy Innovation Hub.

BES sponsored research includes:

- the core BES program with principal investigators (PIs) and their small groups of researchers led by universities or national laboratories;

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

- the EFRCs with their self-assembled groups of 6 to 12 investigators led by universities, national laboratories, and industry; and
- hubs, with a large set of investigators spanning multiple science and engineering disciplines led by national laboratories, universities, nonprofit organizations, or private firms.

Research sponsored by the Advanced Research Projects Agency-Energy (ARPA-E) includes single investigators, small groups, or small teams.

Forty-six EFRCs were awarded, representing 103 participating institutions in 36 states plus the District of Columbia. In FY 11, about $66 million will be competed in the BES program to support single investigators, small groups, and additional EFRCs in (1) discovery and development of new materials and (2) research for energy applications. Awards will be competitively solicited via funding opportunity announcements following the FY11 appropriation. Those solicitations will emphasize carbon capture and advanced nuclear energy systems.

The Cray XT5 computer at Oak Ridge National Laboratory is the biggest, fastest computer in the world and can perform more than 2.3 quadrillion operations per second. One use of the Leadership Computing Facilities (LCFs) is the predictive simulation of combustion in an evolving fuel environment, which is essential for developing more efficient and cleaner engines.

The synchrotron radiation light sources have had a massive impact on structural biology. The winners of the 2009 Nobel Prize in chemistry used all four BES light sources. The newest light source, the Linac Coherent Light Source (LCLS), is having spectacular success.

The Bioenergy Research Centers are starting to demonstrate success, making real progress in developing organisms that can metabolize cellulose directly into ethanol. SC has supported advances in DNA sequencing and analysis that have revolutionized the study of biology. Sequencing the 3 billion base-pair human genome took 13 years. Today the DOE Joint Genome Institute sequences more than a trillion base pairs annually.

The emerging science of high-energy-density laboratory plasma (HEDLP) is enabling a deeper understanding of extreme phenomena in a range of disciplines including fusion energy science, condensed matter physics, materials science, fluid dynamics, nuclear science, and astrophysics.

The Early Career Research Program (ECRP) is up and running. In FY10, 69 awards were funded via the American Recovery and Reinvestment Act; 1,750 proposals were peer reviewed to select the awardees, resulting in 47 university grants and 22 DOE national laboratory awards. Awardees are from 44 institutions in 20 states. Finally, the first SC Graduate Fellowship Program awards will be made in March. We hope that people in this program will get to spend their summers at the national laboratories.

Dr. Brinkman answered questions posed by the panel.

Question: Is the Science for Energy Technology Subcommittee answering the questions that you wanted answered?
Answer: The question was about communication between BES and the industrial community; it needs to be established and maintained. The report does not define extensively how that is to happen.

Question: The Subcommittee had difficulty understanding the charge in the context of the applied technology offices.
Answer: The other offices stay away from the difficult, fundamental research problems. Even ARPA-E is very applied.

Question: How do you get youth interested in energy science and technology?
Answer: That topic is still being talked about. The question is what might be done to change the dynamics. Land-grant-like institutions focused on science and technology might address the need for energy scientists and engineers. Something permanent is needed.

Question: Would there be more hubs in the next 5 years?
Answer: Hubs have been a hard sell. Three now exist, and one is proposed. It will have to be seen how things go with them.

Harriet Kung[2] was asked to give an update on BES and its budget request.

The FY 2011 budget request for BES is $1.835 billion, which is about a 12% increase in real dollars. The major expenditures are for:

- facility operations ($777.3 million),
- Division of Materials Sciences and Engineering (DMSE) research ($309.4 million),
- Division of Chemical Sciences, Geosciences, and Biosciences research ($306 million), and
- EFRCs ($140 million).

The largest increases are for basic research in ultrafast science, materials synthesis, carbon capture, radiation resistant materials, separation sciences, advanced combustion modeling for engine design, geophysics and geochemistry on CO_2/minerals and rocks interactions, and gas hydrates.

Construction funding will include the National Synchrotron Light Source-II, Spallation Neutron Source (SNS) instruments (completing the initial suite), and an SNS power upgrade. The Office's fifth light source, the LCLS at the Stanford Linear Accelerator Center (SLAC) will be fully operational.

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

The FY11 budget request includes about $66 million to support single investigators, small group research awards, and EFRCs in the discovery of new materials and fundamental science for carbon capture and advanced nuclear energy systems. Energy Innovation Hubs are to be initiated in the area of Batteries and Energy Storage and to be continued in the area of Fuels from Sunlight.

An increase in chemical physics enables initiation of a significant effort in the area of multiscale modeling for advanced engine design. An increase in geosciences research enables new research on methane hydrates and various geophysical and geochemical investigations. Increases for ultrafast science research in neutron and X-ray scattering and atomic, molecular, and optical sciences enables development of ultrafast X-ray and optical probes of matter and dynamic phenomena.

Accelerator and detector research is expanded to include free-electron laser, diagnostics, detectors, and accelerator modeling. BES light sources facilities receive funds for critical instrumentation and device upgrades at the Advanced Photon Source, Advanced Light Source, and LCLS at $6 million. The SNS power upgrade project schedule is accelerated.

The Energy Innovation Hub for Batteries and Energy Storage will address a critical issue. It will affect all aspects of energy usage, including consumer products, vehicles, military equipment, and utilities at a variety of scales for such applications as regulation, ramping, peak shaving, and load leveling. Numerous technologies are required for grid and transportation energy storage. These needs are met by a great variety of existing technologies, but those technologies have limited use lifetimes, are far from theoretical densities, have high costs, are often environmentally hazardous, require higher power and charge/discharge rates, and have high weight. For example, current car batteries provide 45 cycles and need to go to 1,000 cycles. Overall, improvements by a factor of 2 to 10 are needed.

The three primary drivers are increased energy density, higher power, and longer lifetimes, leading to the research questions:

- How can we approach theoretical energy densities?
- How do we increase the safe storage capacity and achieve the optimum charge/discharge rate?
- Can we maximize the reversibility?

The Batteries and Energy Storage Hub would address grand science questions that fundamentally limit the cost and performance of a broad range of electrical energy storage applications. The Hub's scope and scale ensure that the technology and production needs would be linked to the fundamental science, resulting in rapid and meaningful communication across the spectrum. It would address the need to strengthen the links from basic science all the way to industrial development and fully integrate consideration of materials selection, architecture design, and manufacturability with systems analysis. The Hub would provide sustained support, allowing the team time for fundamental knowledge and novel concepts to be thoroughly vetted before down-selections are made for applied research and development. The hubs will do high-risk,

high-payoff basic research with government-dominated funding for a relatively long duration.

About $66 million will be competed in the BES Program to support single investigators, small groups, and additional EFRCs in discovery and development of new materials and research for energy applications. New materials discovery is an enabler of technology innovations. Numerous recent Nobel prizes like those for the quantum Hall effect, buckyballs, and conducting polymers were made possible by new materials. The material discoveries have also enabled generations of technology breakthroughs, from integrated circuits, lasers, and optoelectronic communications to solid-state lighting. Further advances in these technologies have been limited by the performance of materials. The science challenge is how to assemble the building blocks of materials.

The discovery of new materials has two goals:

- to develop new synthesis capabilities and a strong foundation for science-driven materials discovery; and
- to build U.S. leadership in materials synthesis and discovery enterprise to drive technology innovation.

The new BES activity will emphasize establishing new synthesis capabilities for materials discovery and synthesis, developing crystalline materials by "reverse design," atom-by-atom design, and exploiting biological strategies and approaches to materials synthesis and assembly.

The 2007 BESAC report, *Directing Matter and Energy*, said that the creation of new materials is an essential component of science grand challenges. The 2008 and 2009 National Research Council (NRC) reports made much the same point. The Office is following that guidance.

The proposed FY11 budget anticipates EFRCs, single PIs, and small groups. The EFRCs are large centers that broadly address materials discovery and crystal growth, provide infrastructure for cutting-edge materials discovery and development, and lend a thematic focus to tackle the most significant synthesis challenges related to energy research. They are complemented by single PIs and small groups that will provide the unique education and training needed for new materials synthesis and discovery and will drive innovation in high-risk, niche research areas. Together, the EFRCs and individual PI activities will result in a network for materials discovery across the nation, building a strong foundation for a culture of science-driven synthesis and providing the scientific and technological impact to return leadership of this crucial field to the United States.

Transportation accounts for 60% of oil consumption, and the combustion engine will be viable for decades to come. But efficiency and cleanliness are difficult to achieve together. Fuel streams are rapidly evolving with new markets for heavy hydrocarbons and new renewable fuel sources (e.g., ethanol and biodiesel). In addition, new engine technologies are being developed. A multiscale simulation of internal combustion engines is directed at predictive simulation of combustion in an evolving fuel environment, which is essential for developing more efficient and cleaner engines. The

scientific community has provided a roadmap. The new BES activity (an additional $20 million) will accelerate the scientific foundation for predictive simulation and modeling design by developing models that span vast scale ranges and improving understanding of fundamental physical and chemical properties. This effort will take a two-pronged approach:

- Computational chemistry and benchmark combustion simulations will be conducted including:
  (1) numerical investigations of canonical flame behavior and automated discovery of chemical reaction mechanisms and kinetics; and
  (2) experimental validation, verification, and discovery.
- Ultrafast Science is being pursued to expand our understanding of chemistry and materials sciences by allowing stroboscopic investigations of the earliest stages of dynamic phenomena. Research directions have been informed by BESAC, NRC, and BES-DMSE reports.

The first experiments have been conducted at the LCLS. The 10- to 100-fs pulses of the LCLS are short enough to resolve processes at the fundamental timescales of electronic and nuclear motion allowing for the discrimination of different electron-electron, electron-phonon, and spin-lattice dynamics. Ultrafast science has a great future.

New staff include Peter Lee, Carlos Sa de Melo, Stephen Tkaczyk, and Jan Hrbek. There are vacancies in Technical Coordination Program Management, Technology Office Coordination, and DOE and Stakeholder Interactions.

The draft BESAC report, *Science for Energy Technology,* has been written. The last paragraph captures the message:

> "The opportunities are large, and the potential impacts on clean-energy technologies and on economic and jobs growth are high. Seizing the opportunity requires maintaining BES's commitment to basic fundamental science, and also finding new mechanisms for BES-funded scientists and industrial scientists to work together in addressing the key scientific challenges of clean-energy development. These collaborations will produce greater understanding and control of sustainable energy conversion at the nanoscale, and faster translation of this knowledge to industry where it can bring emerging clean-energy technologies to competitive viability and transformative impact on our economy."

Dr. Kung answered questions posed by the panel.

Question: How would the EFRCs operate?
Answer: A network of PIs, laboratories, and small groups was envisioned to address the research questions and needs.

Question: Are there specific numbers for major items of equipment (MIE) funding for instrumentation?
Answer: That is in the planning stage and cannot be discussed until construction funding is in hand.

A break was declared at 10:20 a.m. The meeting was called back into session at 11:03 a.m., and **George Crabtree**[3] was asked to report on the Workshop on Science for Energy Technology.

Chairman Hemminger noted that the charge from Dr. Brinkman had been discussed at a previous meeting and that a workshop had been held in January. Two reports, a concept report and a full report, were to be published. The first is to be for policymakers, and the second is to be more technical. He thanked the Subcommittee leadership and membership.

Dr. Brinkman's charge asked BESAC to

1. summarize the science themes that emerged from the BESAC reports 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 the more applied energy technologies;
2. identify how the suite of user facilities can impact basic and applied research on energy, and how industry can access the facilities; and
3. identify other major impediments to successful achievement and implementation of transformative energy technologies.

A Subcommittee was formed. It emphasized industrial participation. It was organized into eight technical panels on solar energy, advanced nuclear technologies, carbon sequestration, electricity storage, electricity delivery, advanced lighting, biofuels, and efficient energy generation and use. Another panel considered DOE user facilities.

Two reports are being prepared. The concept report is intended for wide distribution to decision makers in Congress, the administration, agencies, and the energy community. It is expected to be inspiring, exciting, and high level with a limited number of high-level actionable items. The full report is intended for SC and technically savvy industrial and scientific communities and will have more detailed recommendations and actionable items.

Why reach out to industry? The clean-energy technologies we have now do not work very well. For example, commercial photovoltaics (PV) operate at about 20% efficiency vs. combined-cycle gas turbines, which operate at about 60% efficiency. The reason these technologies have such low efficiencies is that there is no basic science understanding of materials, chemistry, and energy conversion at the nanoscale. Basic science understanding will lead directly to industrial performance innovations. BES can have a huge role in what industry does.

The societal motivation is the traditional economic driver: consumer spending leading to gross domestic product and job growth. Addressing national energy needs and exporting clean-energy technologies to the developing and developed world would build a reliable

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

and enduring new economic foundation. Basic science supporting industry will enable and accelerate this new economic foundation.

Other countries are striving to take the lead in establishing clean-energy technology in Europe and Asia. Other parts of the U.S. R&D enterprise are starting to move into the science-to-industry space [e.g., the National Institute of Standards and Technology (NIST), the National Science Foundation (NSF), and other parts of DOE]. But BES is best positioned to address the need. This is an opportunity to augment the role of BES, but the window of opportunity is short.

From the Basic Research Needs (BRN) Workshop, the process is understood to include grand challenges, discovery science, use-inspired basic research, applied research, and technology maturation and deployment. The first three are traditional BES areas. BES can add the DOE technology offices as clients and provide handoffs to industry. It is not just the *performance* of devices but the fundamental, underlying science that needs improvement.

A number of Priority Research Directions (PRDs) came out of the workshop. Whether they are the *right* directions needs to be discussed. The workshop highlighted the facts that industry sees the value of basic science. The BRNs already identified two kinds of science contributions to energy:

1. "supernovas" (breakthroughs that change the technical landscape like high-temperature superconductivity did in 1986) and
2. understanding and ultimately controlling existing phenomena (a process that is more sustained and that advances in incremental steps).

The SciTech PRDs focused on near-term industry impact. They remarkably echoed many of the BRN PRDs. They emphasize sustained building of the scientific knowledge base underlying technology, like Moore's Law, in which a series of incremental breakthroughs changes the game. Transformational near-term research is possible.

Three overarching themes came out of the workshop:

1. We need to develop a foundational scientific understanding of at-scale production challenges in existing materials and processes.
2. We need to go beyond empiricism to a fundamental understanding of lifetime prediction of materials in extreme environments, especially in aging, degradation, and failure.
3. We need to discover new materials or chemical processes with targeted functionality.

Three crosscutting needs also emerged from the workshop:

1. new materials by design with specific properties or functionalities;
2. the ability to understand, predict, and control interfaces in optical, electrical, mechanical, and chemical behavior; and
3. the understanding of dynamic behavior away from equilibrium.

BES user facilities offer unique resources in structure, spectroscopy, and imaging for nanoscale synthesis and characterization. Facilities could more fully support clean-energy science and specifically industrial-energy science. About 40% of the facilities' time is now used for structural biology, which receives special accommodations in the form of the facility operators running samples sent in by users. The accommodation of quick-response projects is needed for academic, national laboratory, and industry users. Industrial outreach would allow industry to seek industrial advice, perhaps through members of advisory boards. Facility directors and senior managers should seek industry interaction. A portal should be established for industry that attracts users and provides special support. Support staff should be encouraged to engage industry users.

Barriers and solutions can be found in communication, collaboration, and the workforce. Science and industry have differing objectives and styles; science values open publication, and industry keeps knowledge private, rewarding members for performance of products in the marketplace. The workshop was a promising opening to further cooperation.

Science needs to reach out through advisory boards and personal relationships. There could be collaboration in finding challenges that exploit basic science to advance industrial performance by expanding work on the workshop's PRDs and finding the funding incentives/mechanisms needed to promote collaboration. Consortia could be formed for common problems, forming academia–national laboratory–industry exchange programs.

Intellectual property needs a case-by-case solution, and the legitimate needs of both sides must be recognized. Workforce issues include establishing collaborative research projects; student and postdoctoral internships in industry; and exchange visits among universities, national laboratories, and industry.

The discussion at this meeting needs to address three questions:

1. Are these the right messages?
2. Are the messages coming through?
3. How does the Subcommittee follow up?

Dr. Crabtree responded to comments and answered questions posed by the panel.

Comment: Deficiencies have been implied but not described.
Response: Energy technology, more than any other technology, is faced with a problem that requires an understanding of basic phenomena. That needs to be articulated well.

Comment: A large component of the fundamental science community does not know what the emerging questions are. Communication is a key issue.

Comment: This study is to focus on technology opportunities, not BES's structure and operations.

Comment: The fact that industry leaders came and participated was wonderful. They did not know what a user facility was or what BES was. The community is starting off from zero. Industry wants to engage and participate.

Comment: There *are* a lot of new BES facilities that industry does not know about. The report should note that basic science is the only role in this picture. BES funds carbon sequestration at $20 million, but a demonstration project costs $50 to $100 million. BES should address the high-risk research portfolio.

Comment: This workshop should identify initiatives for which money should be sought.
Response: Such initiatives were identified, and they should guide future funding.

Question: How had they managed to get industrial people to attend this 2-day meeting and were the industrial representatives asked how they could get involved with BES?
Response: The industry representatives were gotten there by cajoling them. The second issue was specifically included in the charge to the panels, and there was a lot of discussion about industrial involvement with BES, asking what industry wants from BES. A lot more time could have been spent on those discussions. Industry saw this as a unique opportunity to voice its needs.

Comment: The recommendations look asymmetrical: they say what *BES* can do. They should be balanced with what *industry* can do.

Comment: DOE's Small Business Innovative Research (SBIR) program should be mentioned here. It would be a good starting point.

Comment: The fact that our society really *does* need basic research should be played up in the report.

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

Tuesday, March 2, 2010
Afternoon Session

The meeting was called back into session at 1:34 p.m., and **Alex Malozemoff**[4] was asked for an update on the full report from the Science for Energy Technology Workshop.

The report is a work in progress. The outline has been developed. The publication will have reports from the nine panels, priority research directions, user-facility descriptions, opportunities for strengthening the link between basic research and industry, and recommendations. Since the conference, a panel has been writing chapters of the report; this writing is well under way.

[4] Dr. Malozemoff's full presentation can be found at: http://www.er.doe.gov/bes/besac/Meetings.html#0925

As presently envisioned, the full report amplifies the messages of the concept report, fills in the technical details, and provides a complete discussion of user-facility opportunities and opportunities to strengthen the link between basic research and industry.

The panel reports are up to six pages long but the PRDs are only three pages long. The full report will also have discussions of the PRDs to give additional substance. It has also been suggested that the PRDs be periodically (e.g., annually) updated. Another suggestion is to develop PRDs for each sector in more detail. The big question is whether one can develop and enhance basic research guided by the workshop's PRDs through EFRCs, Innovation Hubs, or new solicitations.

Questions that might be raised about the user facilities include:

- Should clean-energy research be made a priority in a way that is similar to the special accommodations for structural biology?
- Should industry users be given special support?
- Should the proposal-use delay be shortened?
- Can more uniform access procedures be developed?
- Should the scattering and nanoscience centers reach out to clean-energy research and to industry differently?
- Should stronger relationships between facilities and industry be developed, having industry representatives sit on advisory boards, shared events, etc.?

During the ensuing discussion, the panel offered a number of comments and questions.

Comment: Industry tends to view the facilities as being very expensive, and the question was raised whether all expenses were included in the rates for facility use.
Response: Full costs would have to be covered if the work is to be proprietary and not peer-reviewed and published in the open literature. There is a constant reassessment in the costs involved in different uses.

Comment: The cost of doing proprietary research could be looked at. Running an experiment at the LCLS would cost $0.5 million. But there is not uniformity from facility to facility in the way charges are levied.

Comment: The allocation of facility resources to industry as well as to scientists should require review of scientific merit. Industry should step up to support beamlines for, say, materials, as do the biologists and pharmacologists. Facilities have user groups, and industrial members could be invited to attend user-group meetings.

Comment: The one-size-fits-all issue arises at the SNS, too. With powder diffraction, one can run multiple samples on one beamline run. One cannot do that with spectroscopy.
Response: The science–industry link could be strengthened through collaboration, forming consortia, exchange programs, and resolving intellectual-property issues (e.g., by identifying a standard framework for agreements.

Question: Were lessons to be learned in the report?
Response: The Semiconductor Research Corporation was one such lesson.

Comment: There needs to be a bigger awareness of energy in all its forms in an integrated manner. The workforce issue is a big one. Universities, BES, and the national laboratories can all address that issue.

The Subcommittee's next steps are to have the concept report finalized and issued in March. The full report draft is to be completed in April/May and presented to BESAC August 5-6. The Subcommittee also needs to brief SC, perhaps before completing the full report. It then needs to conduct outreach to DOE-BES, the technology offices, the user facilities, upper management, congressional staffers, industry, and wider technical and nontechnical audiences.

Eric Rohlfing[5] was asked to give an update on the energy innovation hubs, particularly the Fuels from Sunlight Hub.

Dr. Rohlfing noted that the first Energy Research and Development Administration (ERDA) Solar Photochemistry Research Conference was held in 1977. The 31st DOE Solar Photochemistry Research Meeting was held in June 2009. The BES Council on Chemical and Biochemical Sciences Workshop on the Efficiency of Photosynthesis was held May 23-24, 2009. It examined whether biologists studying natural photosynthetic systems could talk to physical scientists doing PV research? The answer was yes, and usefully.

The solar energy conversion efficiency of natural photosynthesis is not great. One starts with 1000 W from the Sun and ends with 46 kJ from C3 plants and 60 kJ from C4 plants. The theoretical efficiency of photosynthesis conversion to biomass is 4.6 to 6.0%, but the actual value is 2.4 to 3.7%. Photon capture and energy transfer occurs in femtoseconds, charge separation and electron transport in picoseconds to nanoseconds, and catalysis and fuel formation in microseconds to milliseconds.

The critical research issues for the Energy Innovation Hub, Fuels from Sunlight, are:

- In photon absorption and harvesting: How does one control light harvesting to use all of the photons?
- In charge separation and transport: How does one avoid recombination of photo-generated charge carriers?
- And in photocatalysis: How does one produce fuels with the energy provided by visible light absorption?

Today, one can use a PV cell to produce current in an electrolyzer to produce hydrogen gas as a fuel. What is desired is to use solar microcatalytic energy conversion to directly make a liquid for fuel. There are different ways to plug into solar fuels production. The landscape for solar fuels is pretty much covered by the EFRC areas of focus. What is needed is an integrating effort. This will be provided by the Fuels from Sunlight Hub.

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

This hub is part of a significant new DOE initiative, one of three hubs funded at $22 million each in the FY10 appropriation.

The key dates for the Fuels from Sunlight Hub are:

- Dec. 22, 2009, when the Funding Opportunity Announcement (FOA) was issued;
- Jan. 29, 2010, when the letters of intent were due;
- Mar. 29, 2010, when the full applications are due;
- June 2010, when the awards will be announced; and
- August 2010, when the awards will be initiated.

The objective of the Fuels from Sunlight Hub is to develop an effective solar-energy-to-chemical-fuel conversion system. The system should operate at an overall efficiency and produce fuel of sufficient energy content to enable transition from bench-top discovery to proof-of-concept prototyping. The scale, efficiency, etc. are not being specified. This is clearly a high-risk/high-payoff enterprise. In the scheme of research, from grand challenge to discovery to use-inspired to applied to marketable product, only solar hydrogen has transitioned to the applied status. Light absorption, charge separation, and transport; dark catalysis; nanobiocatalysis; and separations are still in the earlier stages. With the Fuels from Sunlight Hub, integrated solar fuel systems will be developed, creating the scientific and technical infrastructure for a solar fuels industry.

There is a Hub Working Group [including SC/BES, Nuclear Energy (NE), and Energy Efficiency and Renewable Energy (EERE)] that coordinates hub activities and makes recommendations to DOE senior management. Some of its tasks include development of three separate FOAs from a common template; developing a hub cost-sharing plan; allow eligibility for non-DOE federally funded research and development centers [FFRDCs (e.g., NIST and the Jet Propulsion Laboratory)] and foreign institutions to act as partners (not leads); post a hub website and coordinate updates; and coordinate the hub merit-review process. The website gives an overview of the hub program; tells how to apply, includes links to FOAs; describes the research areas; and answers frequently asked questions.

In the Modeling and Simulation of Nuclear Reactors Hub (NE), the FOA was issued January 20, 2010; full applications are due March 8, 2010. Its mission focus is to apply existing modeling and simulation capabilities to create a user environment that allows engineers to create a simulation of a currently operating reactor that will act as a "virtual model" of that reactor. The Hub will also obtain data from that existing reactor to be used to validate the "virtual model."

In the Energy Efficient Buildings Design Hub (EERE), which includes funding from the Department of Commerce, Small Business Administration, Department of Labor, Department of Education, and NSF, the FOA was issued on February 8, 2010; full applications are due on May 5, 2010. This pilot initiative will spur regional economic growth while developing innovative energy-efficient building technologies, designs, and systems.

The response of letters of intent (LOIs) for the Fuels from Sunlight FOA was very positive. A lively competition with strong applications is anticipated. For the EFRC competition, finding unconflicted peer reviewers will be a challenge. Suggestions or volunteers from BESAC regarding peer reviewers are welcome.

Dr. Rohlfing answered questions posed by the panel.

Question: How will there be industry cooperation with BES when there was nothing close to a technology?
Answer: One needs to determine whether there are any showstoppers, and industry is the sector with the best experience in this.

Question: Are there were any requirements to use CO_2-producing fuels to address global warming?
Answer: It is not required, but it is expected that they will be used.

Dr., Hemminger declared a break at 3:23 p.m. The meeting was called back into session at 4:06 p.m. **Altaf Carim**[6] was asked to present an update on the EFRCs.

The research proposed in an EFRC application must address:

(1) one or more of the challenges described in the BESAC report *Directing Matter and Energy* and

(2) one or more of the energy challenges described in the ten BES Basic Research Needs workshop reports.

Forty-six centers have been awarded to 100 participating institutions in 36 states plus the District of Columbia. The EFRC management team is made up of members from all three of BES's divisions plus a representative from BES Operations. Periodic directors' meetings are being held, and reverse-site peer reviews are coming up soon.

The website has been revised. It now includes a compilation of two-page EFRC technical summaries and information on the FY11 funding for EFRCs. A technical summaries book and a single-slide synopsis for each EFRC are also available.

The monthly teleconferences by EFRC subgroups have evolved from being largely administrative discussions to having more science content and discussion. The second EFRCs' directors' meeting was held the day before this meeting with 130 attendees. Management from DOE program managers discussed updates, communications issues, upcoming management reviews, and facilitative mechanisms. Topical breakout sessions dealt with interactions and information exchange among EFRCs and other offices within DOE.

Contractors' meetings provide a key opportunity for EFRCs to benefit from related work supported in the BES core programs and vice versa. EFRC representatives have already been participating in a number of the ongoing BES contractors' meetings, including the

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

2009 Condensed Phase and Interfacial Molecular Science Research Meeting and the 2009 Synthesis and Processing Contractors' Meeting. BES is trying to balance the benefits and desirability of involvement of EFRCs in such meetings with the need to avoid overburdening the centers with such requests.

Early-stage management/operations reviews will be held in spring/summer 2010. Each one is a half-day meeting in the greater Washington area for each EFRC. Participants include key EFRC personnel, BES program managers, and three to five external reviewers. The purpose is to help each EFRC get the best start possible. They will focus on leadership, management, and operational practices and address best practices and operational issues. Guidance and instructions for preparation of review documents have been disseminated. It would be helpful to disseminate management reference documents to the EFRCs. Three have been disseminated so far: Acknowledgements, Annual Progress Reports, and Change Controls.

Dr. Carim responded to questions posed by the panel.

Question: What worked and what did not work?
Answer: It has been surprising how quickly these centers have gotten out of the gate. They ramped up personnel rapidly. Internal-communication issues have been problematic, and many types of solutions are being tried. A funded activity has already made a journal cover. The interactions with the technology offices have been a pleasant surprise.

Question: Have there been any issues on getting the money out to numerous institutions.
Answer: That had happened quickly for some and longer for others. There were not many delays, and there was not anything systematic to the delays. The awards were given out when it had been said they would. The visibility of the program helped getting the awards through the contracting office. Processes are different for different universities; that may have been a cause of the few delays.

Question: Is the whole were greater than the sum of the parts of the EFRCs in terms of science production?
Answer: Yes. A lot of cross-pollination is going on.

Question: Is this an opportunity for strengthening the link between BES and industry.
Answer: There is the possibility, and some EFRCs are already pursuing ties with industry. Some EFRCs have industry partners.

Dr. Hemminger reopened the discussion of the Science for Energy Technology Workshop and its reports. Issues raised or comments made in earlier discussions of the concept report included

1. There is a difference between PRDs from the BRNs and those from the Science for Energy Technology Workshop process.
2. In the report as written, the need for this to be a two-way street needs to be stressed. Industry engagement would be very helpful.

3. The premise of the report must be made clearer.

The panel asked if there would be funding for the issues identified in the Science for Energy Technology Workshop. Chairman Hemminger suggested that perhaps not all the money should come from DOE. This workshop generated much interest. That interest should sustain additional interaction and communication. The same questions could have been raised about each BRN. How to go from identifying a problem to getting money to address the problem could be treated in the full report.

The panel suggested that it would be helpful to articulate the nature of basic research and how strategically important it has been. It is the headwaters. One can improve the short-term benefits of long-term research by tightening up relationships with industry. The chairman agreed; doing fundamental research is the role of BES. He suggested listing the four shortcomings of the concept report and having the cochairs implement those changes. It was so moved and seconded. The motion passed unanimously. Hemminger asked for volunteers to review the revised draft. McCurdy, Richards, and Greene volunteered.

Celia Merzbacher agreed to give a presentation on the following morning on how the Semiconductor Research Corporation works. That item was added to the morning's agenda. All members were charged to review the Malozemoff presentation on the full report and to come prepared to discuss that report during the following day.

The floor was opened to public comment. There being none, the meeting was adjourned for the day at 4:53 p.m.

Wednesday, March 3, 2010
Morning Session

The meeting was called back into session at 9:08 a.m. **Celia Merzbacher** was asked to describe how the Semiconductor Research Corporation (SRC) operates. It funds basic research at universities. It was founded in 1982 as a consortium of semiconductor companies to fund and manage university research. It defines relevant research directions, explores potentially important new technologies, and generates a pool of experienced faculty and relevantly educated students. It reviews proposals and awards grants.

Since 1982, SRC has funded $1.3 billion in basic research under 2,906 contracts with 241 universities in 60 countries. It has produced 43,419 technical documents, 326 patents, and 2315 research tasks/themes. Member-company liaisons give advice to the university researchers, transfer the research results to companies that need them, and mentor the students.

The SRC was formed to bolster relevant education for the members' workforce. Today, SRC funds 500 faculty and 5,000 students annually. It has four programs:

1. The Global Research Collaboration, with 5-year contracts on traditional complementary metal oxide semiconductors (CMOS).
2. Focus Center Research Programs, with 5- to 10-year contracts probing the limits of traditional CMOS and funded 50-50 with the Defense Advanced Research Projects Agency (DARPA).
3. Nanoelectronics Research Initiative, with longer than a 10-year horizon to look for revolutionary discoveries beyond CMOS with DARPA and state participation.
4. Emerging Initiatives, with various horizons for selected topics.

SRC leverages investments by fierce competitors, is industry-driven, and is flexible and responsive. Its attributes include:

- it connects researchers in the university community, and university researchers with industry experts;
- it provides access to the best faculty and students in the field, has built a broad university network with established practices;
- it develops a top-notch future workforce;
- it provides the infrastructure and processes for delivering information;
- it offers efficient management, and maintains federal partnerships for mutual benefit (with DARPA, NIST, and NSF).

SRC has a long-term contract with DARPA to fund the research centers. Federal agencies sit on the review panels. It augments NSF investments in certain areas. It releases joint solicitations with NSF, resulting in two research contracts per award, one from SRC and one from NSF. Results from selected NSF research efforts are disseminated by SRC to its members.

The panel had several questions for Dr. Merzbacher.

Question: How does one jump start such an industry consortium?
Answer: The willingness to work with a competitor is difficult to bring about, and small companies may not have the resources to participate. A business-to-business conversation is the best way.

Question: What are the contrasts between the SRC funding and government funding?
Answer: SRC funding is quick, going from proposal to contract in a month. The contracts lead to jobs for students.

Question: What is the total budget for SRC?
Answer: $100 million per year.
Question: Could one get an exclusive license when royalty-free licensing was offered?
Answer: A lot of cross-licensing was done. Universities own the intellectual property and can license it as they wish.

John Spence was asked to present an update on experiments at the LCLS. The LCLS is the world's first hard X-ray laser. Femtosecond X-ray nanodiffraction analyzes single-protein crystals 30 times a second. It provides good spot patterns. Fine spectra give new

information. One can find the distance between facets of submicron crystals by counting fringes. A snapshot from a single virus can be inverted to produce an image with 200-Å resolution.

The diffract-and-destroy process works at high resolution on delicate membrane proteins. Submicron nanocrystals in solution can be solved. This opens the way to dynamic studies. 3-D constructions are obtained from 2-D information. There is no evidence of radiation damage between 3 and 200 femtoseconds at 8-Å resolution.

Julie Carruthers[7] was asked to present an overview of the SC Graduate Fellowship Program. The purpose of this program is to support outstanding students pursuing advanced degrees in basic research and to encourage the development of the next generation of scientific and technical workforce in the United States. In FY10, about 160 awards will be made. The $5 million appropriated will support the first year for about 80 graduate fellows, and $12.5 million from the Recovery Act will forward-fund about 80 graduate fellowships for 3 years. The FY11 request is $15 million. This $10 million increase will support a new cohort of about 170 students.

The Office of Workforce Development for Teachers and Scientists (WDTS), in consultation with the SC Office of the Deputy Director for Science Programs, developed the program plan and schedule. The Oak Ridge Institute for Science and Education (ORISE) is providing administrative support for the peer review of applications and administration of awards. A working group of SC program managers was established to provide technical input and assistance with the peer review of applications.

The fellowship is a 3-year award, totaling $50,500 per year. It includes a $35,000 annual living stipend, $10,500 towards tuition and fees, and a $5,000 annual research stipend. Each year WDTS will hold a summer research conference at one of the DOE national laboratories. The conference will provide an opportunity for fellows to present their research. It will also serve as an orientation for new fellows, offer guest lectures, tours of the host laboratory, professional-development seminars, and workshops on how to access the DOE user facilities and collaborate with national laboratory researchers.

Eligibility requires applicants to be a U.S. citizen, a senior undergraduate or first- or second-year graduate student, and be pursing an advanced degree in areas of basic research important to the SC and DOE missions. The application asks for academic history, awards, publications, two essays, transcripts, and three letters of recommendation.

The peer review process was developed to handle 8,000 to 10,000 applications. There was an eligibility and compliance review, and now each application is receiving three independent reviews by subject matter experts in the applicant's area of proposed graduate research. The top 500 to 600 applications will be selected to be the focus of the onsite merit-review panels to evaluate fellowship applications across the scientific disciplines based on the established merit-review criteria.

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

SC program manager participation is integral to the execution of the program in its inaugural year. Expert program managers were nominated by their associate directors with two or three program managers from each SC program participating in the working group. Program managers provide valuable technical advice on the peer-review process and have reviewed applications in the eligibility review, recruited and selected reviewers for the online and onsite reviews, and served as proctors for the online and onsite reviews.

Selections for the FY 2010 program are expected to be announced at the end of March. A committee of visitors (COV) will evaluate the process in May and make recommendations for improvement for the 2011 program. The FY11 call for applications will be issued in the fall of 2010.

The panel had several comments and questions for Dr. Carruthers following her presentation.

Comment: The online review was impossible to navigate.
Response: There have been a lot of lessons learned and improvements will be made next year. Because of the rapid timeline, the process was not fully tested across all platforms.

Question: Can students who were not successful reapply next year?
Answer: Yes.

Dr. Hemminger reopened the discussion of the reports from the Science for Energy Technology Workshop. He stated that further engagement by the Committee was needed in the process of documenting this workshop as the front portions of the report(s) are written. All Committee members should be responsive when they hear from the workshop chairs. He urged the Committee members to look for things that need clarification or things that are missing.

Malozemoff said that feedback will be sought on the more generic chapters. Individual reviewers for each of the topic-specific (technical) chapters are also being sought. There are also chapters on barriers and solutions, PRDs, and user facilities.

- Greene volunteered to review electricity delivery.
- Flynn was volunteered to review solar energy.
- Tranquada volunteered to review advanced nuclear.
- Cummings volunteered to review carbon sequestration.
- Taylor volunteered to review electrical storage.
- Spence volunteered to review advanced lighting.
- Gates and Richards volunteered to review biofuels.
- Taylor volunteered to review efficient energy generation and use.
- Berrah and Tranquada volunteered to review user facilities.
- Everybody was encouraged to review the list of opportunities.

The floor was opened for public comment. **Alan Hurd** noted that Los Alamos National Laboratory has been accommodating national-security people in neutron scattering for years. With national-security applications, a score of up to 20% extra is assigned above the general-access proposals. That programmatic score has been shaved back to 10%. There is an opportunity cost for every proposal, and it varies by instrument used. Outreach is needed to industry because industry under-appreciates the benefits of neutron scattering. This outreach is expensive, but it leads to growth in usage, although an upswell in industrial participation has not yet been seen.

David Miller said that all offices have roadmaps that point to research needs out to 10 or 20 years. Program managers should look at roadmaps within industry groups.

There being no further public comment, the meeting was adjourned at 11:00 a.m.

Respectfully submitted,
Frederick M. O'Hara, Jr.
Recording Secretary
April 6, 2010
(Edited 4/19/10 MIS)