Minutes of the
Basic Energy Sciences Advisory Committee Meeting
August 3-4, 2006
Marriott North Bethesda Hotel and Conference Center,
Bethesda, Maryland

BESAC members present:

Nora Berrah
Sylvia Ceyer
Sue Clarke
Peter Cummings
Frank DiSalvo
George Flynn
Bruce Gates
Laura Greene
John Hemminger, Chairman
Eric Isaacs
Anthony Johnson
Walter Kohn
Gabrielle Long (Thursday only)
William McCurdy, Jr.
Daniel Morse
Martin Moskovits
Ward Plummer
John Richards
John Spence (Friday only)
Kathleen Taylor
Mary Wirth

BESAC members absent:

Mostafa El-Sayed
Kate Kirby
Stanley Williams

Also participating:

Kristin Balder-Froid, Physical Biosciences Division, Lawrence Berkeley National Laboratory
Linda Blevins, Office of Basic Energy Sciences, USDOE
George Crabtree, Director, Materials Science Division, Argonne National Laboratory
Patricia Dehmer, Associate Director of Science for Basic Energy Sciences, USDOE
Graham Fleming, Associate Laboratory Director for Physical Sciences, Lawrence Berkeley National Laboratory
Jay Groves, Physical Biosciences Division, Lawrence Berkeley National Laboratory
Harriet Kung, Office of Basic Energy Sciences, USDOE
Tobin Marks, Department of Chemistry, Northwestern University
Paul McEuen, Department of Physics, Cornell University
Terry A. Michalske, Director, Center for Integrated Nanotechnologies, Sandia National Laboratories
John Miller, Chemical Sciences, Geosciences and Biosciences Division, Office of Basic Energy Sciences, USDOE
Pedro Montano, Director, Scientific User Facilities Division, Office of Basic Energy Sciences, USDOE
Teri Odom, Department of Chemistry, Northwestern University
Frederick M. O'Hara, Jr., BESAC Recording Secretary
Raymond Orbach, Under Secretary for Science, USDOE
Julia Phillips, Director, Physical, Chemical, and Nano Science Center, Sandia National Laboratories

Mark Ratner, Department of Chemistry, Northwestern University
John Sarrao, Condensed Matter and Thermal Physics Group, Los Alamos National Laboratory
Leslie Shapard, Oak Ridge Institute for Science and Education
Karen Talamini, Office of Basic Energy Sciences, USDOE

About 90 others were in attendance in the course of the two-day meeting.

Thursday, August 3, 2006
Morning Session

Chairman John Hemminger called the meeting to order at 8:38 a.m. **Leslie Shapard** made convenience and safety announcements. Hemminger had the members introduce themselves and then called upon **Patricia Dehmer** to give an update on the Office of Basic Energy Sciences (BES).

The Spallation Neutron Source (SNS) project is complete. In 1996, BESAC set the technical specifications of the SNS, and ground breaking occurred in December 1999. The paper indicating project completion was signed on June 5, 2006. During the next few years, about 12 instruments will be commissioned, and about 6 more are expected. BESAC's recommendations had a great influence on the design and power of the facility.

Construction is complete and initial operations are under way at four Nanoscience Research Centers (NSRCs), and the one at Brookhaven National Laboratory is under construction. Soon, all will be operational. BESAC played an important role in getting these centers started and in determining what user community would be served and how.

The FY06 appropriation for BES was $1.135 billion. The President's FY07 budget request was $1.421 billion, an increase of $286 million. Both the House and the Senate have produced markups of the budget. The House mark is the same as the President's budget request. The Senate mark increases the budget request by $25 million. This is an enormous increase. Now there will be a reconciliation of these two markups.

BESAC has held a series of Basic Research Needs (BRN) workshops during the past 4 years. BESAC chartered the BRN Workshop on a Secure Energy Future, which considered all energy sources and technologies. The weeklong workshop's major recommendation was, "considering the urgency of the energy problem, the magnitude of the needed scientific breakthroughs, and the historic rate of scientific discovery, current efforts will likely be too little, too late. Accordingly, BESAC believes that a new national energy research program is essential and must be initiated with the intensity and commitment of the Manhattan Project, and sustained until this problem is solved." A number of follow-on workshops were held on

- the hydrogen economy (a huge success that resulted in funding for hydrogen research and precipitated a number of professional-society symposia and 700 preproposal submissions);
- solar energy;
- superconductivity;
- solid-state lighting;
- advanced nuclear-energy systems;

- clean and efficient combustion of transportation fuels (upcoming); and
- geosciences (upcoming).

Past and future BRN workshops will consider carbon-energy sources, carbon management, no-net-carbon energy, energy distribution and storage, and energy consumption. They will also try to address the uncertainties associated with hydropower, biomass, geothermal, wind, solar, and ocean energies. Cross-cutting workshops are also being considered on catalysis and materials under extreme conditions.

These workshops have been asked to look at relationships between the science and technology offices in DOE. They start with the boundary conditions so the research comes with the goal of meeting technical milestones, with emphasis on (1) the development, performance, cost reduction, and durability of materials and components or efficient processes and (2) proof-of-technology concepts. The workshops identify technology maturation in terms of scale-up research, at-scale demonstration, cost reduction, prototyping, manufacturing, and deployment support. The workshops then develop use-inspired basic research [basic research for fundamental new understanding, with the goal of addressing short-term showstoppers on real-world applications in the energy technologies (e.g., materials for hydrogen production)]. As well, they look at long-term discovery research: basic research for fundamental new understanding (i.e., science grand challenges) on materials or systems that may be only peripherally connected or even unconnected to today's problems in energy technologies and the development of new tools, techniques, and facilities, including those for advanced modeling computation. The findings can be summarized in a four-column chart under discovery research, use-inspired basic research, applied research, and technology maturation and deployment.

The workshops have done a good job at interrelating BES research with applied-technology offices' needs. In applied research, one milestone is to develop, by 2025, advanced solid-state lighting technologies with a product system efficiency of 50% with lighting that accurately reproduces the sunlight spectrum. The workshops have identified use-inspired basic research on (1) computational design and synthesis of unconventional light-emitting materials with tailored properties, (2) the discovery of design rules for robust photon-conversion materials and matrices for use in the UV-visible-IR spectrum, and (3) managing and exploiting disorder in organic light-emitting devices. In discovery research (which holds the next challenges for BES to provide a foundation for use-inspired basic research), the workshops identified as needs (1) understanding and controlling radiative and nonradiative pathways in semiconductors, (2) new functionalities through heterogeneous nanostructure, (3) innovative photon management, and (4) enhanced light-matter interactions.

As a result of these BRN activities, in FY07, core research will be up $8.8 million, hydrogen fuel will be up $17.5 million, solar-energy utilization will be up $34.1 million, advanced nuclear-energy systems will be up $12.4 million, and all others will be up $30 million.

Two solicitations are out now, one for basic research for the Hydrogen Fuel Initiative and one for solar energy utilization (based on findings from the workshop). In solar-energy utilization, 656 preproposals have been received, and the requests for full proposals were to go out the week following this meeting. All of this new work is a fabulous success for BES.

During the past 6 years, SNS construction has driven the construction portion of the BES budget. From 2005 to 2007, the facility-operations section of the budget is increasing significantly, a direct influence of the American Competitiveness Initiative (ACI) and the opening of the NSRCs and other user facilities. After a decrease in FY06, the research section of the budget is resuming its historical increase, largely driven by the ACI. A major challenge faced by the Office is to understand how to manage such a portfolio and support a depth and breadth of research sufficient to meet the challenges of the future.

The four-column chart used to represent relationships among the science and the technology offices in DOE implies the existence of a fifth column of unknown future challenges, which must also be considered, especially by BESAC.

Gates asked what the participation by industry has been in the workshops and what will happen in the future. Dehmer said that industry had participated in all the workshops and breakout sessions. This participation will continue.

Cummings asked what the “NNI portfolio” was. Dehmer replied that these are the ongoing programs from the National Nanotechnology Initiative (NNI).

Richards noted that some $128 million was taken out of the budget of the Office of Biological and Environmental Research (BER) and asked what happened to it. Dehmer answered that those fund were for Congressionally mandated directives, about 80 of them. Those are automatically withdrawn. Congressional directives are for 1 year only. BES has $25 million in Congressional directives in the Senate markup, some $6 million of which are unfunded. (BES will have to fund them if they remain unfunded; the hit will likely be spread across all of BES.)

Moskovitz observed that DOE’s plans have always exceeded its budget and asked what had not been done in the past that would have been wonderful to do. Dehmer responded that facilities and long-term and basic research both have more to do, such as in solid-state lighting and energy storage. Research that will affect energy systems also needs to be done (e.g., on radiation effects on materials). All of SC could easily double its budget.

Greene stated that the core budget seems to be decreasing. Dehmer agreed that that is correct. The workshops were so successful that funding is flowing into those programs touched by those workshops.

Kohn noted that Nakamura won a prize in technology for solid-state lighting.

Richards said that Dehmer and her staff are to be commended for producing these increases in funding.

Frank DiSalvo was asked to report on the Committee of Visitors (COV) to the Division of Materials Sciences and Engineering, one of the three divisions in BES. The COV was held April 3-5, 2006. The charge was to (1) review activities of the Division of Materials Sciences and Engineering within BES, both the laboratory and university projects, and to assess the efficacy and quality of processes used to solicit, review, recommend, and document proposal actions and (2) monitor active projects and programs. The COV was also to comment on (1) how the award process has affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements and (2) the Division’s contributions to the long-term goals of BES.

The COV’s 28 members were broadly distributed in subject specialty, institutional affiliation, and funding source. No panel members were from Experimental Program to

Stimulate Competitive Research (EPSCoR) states, but that was not considered to be a problem.

The FY07 budget request for this Division is $287 million, a 26.5% increase over the previous year. The Division is organized into two teams with four research activities. The COV reviewed six groups: Structure and Composition of Materials; Mechanical and Physical Behavior of Materials; Synthesis, Processing, and Engineering Sciences; X-Ray and Neutron Scattering; Condensed-Matter Physics; and Materials Chemistry and Biomolecular Materials. 29% of the research funding of these activities goes to university grants; 71% of it goes to national-laboratory field work proposals (FWPs). The number of grants is much greater than the number of FWPs. The average size of a grant is $150,000 per year; the average FWP is $1.5 million. The total 571 projects is a large number to keep track of.

The COV was given overviews, was split into six subpanels, performed a first reading of folders (especially those at the margins), was redistributed into seven subpanels, performed a second reading of folders, and wrote a report. The 2003 COV made several recommendations, and the following responses were made by the Division to those recommendations:

- The difficulty for program manages to use a database is unresolved.
- A reviewer database has been established.
- The need for the collection of anonymous principal investigator (PI) data is unresolved.
- A timeline page has been implemented in the folders.
- Better PI unification has been accomplished to some degree.
- Extra resources have been allocated to support travel by program managers to meetings and laboratory visits.
- The size of grants has been increased by 7%.

The current COV found that the research being funded by the Division is both centrally relevant to the DOE mission and of exceptionally high quality. In particular, there was resounding affirmation of the quality and soundness of the program managers' decisions to fund or not fund. The program managers do have some latitude and freedom in making such decisions and have exercised that freedom with wisdom and responsibility. The COV strongly affirmed the degree of discretion given to program managers, especially when some oversight by a COV is in place to verify continued good judgment.

A particular concern was the very large workload of the program managers. Staffing levels reached a low of 60% of normal. However, even at full complement, the staffing of the Division is likely to be too low in the near future. A requested increase of 26% in the BES budget will increase that workload, and similar increases in budget can be expected in subsequent years. Two changes in program management and strategy instituted in 2006 will require more staff time: coupling of the BES program to the technology areas and instituting an open-door policy for PIs to visit program offices. Program managers have been unable to attend scientific meetings, visit PIs, and keep informed about opportunities at the forefront of science. The number of supported proposals in the total budget managed by each program manager is large because of the large number of university grants. SC should begin planning to meet these needs before crisis sets in again.

A very large issue is information management. This problem was also identified by the 2003 COV. Although some progress has been made, much remains to be done. The current COV considers information management to be the second most important problem faced by the Division after staffing. The resources and staff should immediately be allocated to implement comprehensive and effective information management within SC.

The BRN workshops carried out by BES have been a huge success. They have galvanized the research community to take on grand challenges and have been an important tool for SC in communicating the mission and goals of BES to Congress and the Office of Management and Budget (OMB). Those workshops should be continued and expanded.

The COV strongly supported the decision by BES to fold initiatives into the dynamically managed core research areas. This mode of management has been very effective.

The full portfolio of supported research is divided between multi-investigator programs at the national laboratories and single-investigator programs at universities in a ratio of approximately 70% to 30%. The supported research in both cases was considered world-class. It is notable that, in recent initiatives, the ratio of support is closer to 50-50. It appears that this ratio arose purely on the merits of the proposed research. The COV supported the notion that university research support should generally be in the form of single-investigator grants. However, when appropriate, and as is done on a small scale already, multi-investigator grants at universities can be an important tool to attack key areas, especially those identified with grand challenges in energy research that require an interdisciplinary team approach. Teams that come and go as the needs, challenges, and funding evolve were considered more appropriate. Such teams may also lead to a greater interaction between university and laboratory researchers, as dictated by the needs and opportunities inherent in the research. Perhaps some could even be jointly funded. The COV supports the idea that the balance of support between laboratories and universities be determined by open competition wherever and whenever feasible. The COV suggests that BESAC be used as a sounding board as the details of university-based multi-investigator programs are explored and developed.

The EPSCoR Program was evaluated separately and only reviewed in the second reading. The process of soliciting, reviewing, recommending, and documenting proposal actions was uniformly applied within the context of the EPSCoR-defined boundaries. However, monitoring of the projects and programs is spotty. The state-originated reports from implementation grants lacked details and, in general, were not convincing. There are no metrics for success in this program. The monitoring of the Laboratory Partnership Grants of EPSCoR is much better. While the EPSCoR objectives were addressed in the proposals, the level of monitoring to assure progress toward the objectives is inadequate. This is not caused by the lack of diligence of the program manager but rather by an absence of any metrics to measure effectiveness. BES should consider coordinating an interagency assessment program for EPSCoR. However, the Laboratory Partnership Program has been quite effective in accomplishing this objective.

OMB’s Program Assessment Rating Tool calls for the Division to achieve four goals by 2015, and the COV was asked to rate the Division’s progress on these goals. The

Program Assessment Rating Tool (PART) ratings by all six subpanels were “excellent” in all relevant areas.

Greene asked if the 450 grants per year were 450 PIs. DiSalvo replied that these include multiple PIs but not the University of Illinois grant. So that is approximately 450 people supported. The new proposals coming in vary from year to year. Greene asked what percentage of the 350 proposals is actually funded. DiSalvo answered that renewal proposals are granted at a rate of 80% and new proposals at 25 to 30%. Greene asked what “bulk grants” are. DiSalvo said that he meant multi-PI grants and the opportunity for additional collaboration. The COV did not get into how the money is managed.

Plummer noted that only one state has ever graduated out of EPSCOR, so it seems to be a failure. DiSalvo replied that some say that it is successful because so many states have been added. Plummer asked if there was someone who screens proposals for formats and completeness. DiSalvo replied that there is no rigid format for proposals. Kung added that that is true for all of SC, although reviewers have specific information needs. Plummer asked if the COV had looked at how referees for proposals were chosen, specifically the percent of reviewers who were funded by DOE. DiSalvo answered that this question had not come up. Hemminger said that the reviews were seen to be conducted in an appropriate manner and the quality of reviewers was high.

Berrah asked if national-laboratory grants were reviewed in the same way as university grants. DiSalvo said that the ways they are reviewed are not wildly different. The national-laboratory grants, once made, are renewed more frequently than university grants are.

Ceyer asserted that it is necessary for the core research to evolve and stay relevant. DiSalvo agreed that those programs are evolving and need to continue to do so.

Kohn asked to what the 70% to 30% split refers. DiSalvo responded, budget. Kohn asked what the average support of a single PI at the national laboratories is. DiSalvo said that he did not know. Kung stated that a one-to-one comparison cannot be made. The average support for a PI at a national laboratory would probably be larger. Kohn asked whether, for decisions at the margin, there are any procedures for rejectees to get a second review and whether it is a significant problem. DiSalvo replied that many good proposals do not get funded because of lack of money. Program managers make those decisions and do a great job at it. PIs of proposals that are ranked low are given the opportunity to critique the evaluation.

Gates asked if the COV was tempted to make a recommendation about the influence of inflation’s increase on overhead expenses in university grants. DiSalvo said that the COV did not have enough time to seriously consider that problem. BESAC may want to address that problem.

Moskovitz noted that, over the years, support for energy research at universities has declined. They have a role to play; they have not been able to make their case. A meeting should address how universities could play a better role in advancing DOE’s mission and mandate. Dehmer noted that, when SC puts out solicitations, it limits the national laboratories’ submissions so they are prescreened and therefore are more likely to be successful. Workshops are held on scientific topics to engage the broad scientific community. A workshop of senior university administrators might be held to explore how they could get their institutions more engaged.

Cummings pointed out that most national-laboratory projects have university subcontractors. Grants.gov is an inequity being visited on researchers. Dehmer noted that that is all coming from above.

Hemminger asked for approval of the report; there were 13 votes for accepting it and 4 abstentions. A break was declared at 10:50 a.m. The meeting was called back into session at 11:15 a.m. Hemminger said that, over the years, each COV has pointed out the lack of demographics available on grants made by BES. He introduced **Linda Blevins** to describe the roadblocks that SC faces in collecting demographic data on the people with whom it interacts. The term "demographic" refers to career stage, gender, and ethnicity. Eight out of eleven COVs have asked for this capability.

As a leader in funding the physical sciences and a steward for the national laboratories, SC has a responsibility to manage its programs in the most professional way. It is also DOE policy to foster a culture of inclusion and respect that values, embraces, and promotes diversity in everything the Department does.

A proposal submitted to SC starts with a PI, goes through a common portal (grants.gov), and is entered into an interactive procurement system. All of this information is saved by SC staff members on a common hard drive. Key data from the proposal go into the system, Information Management for the Office of Science (IMSC). DOE information-technology databases cannot collect demographic data because they are not systems of records. A system of records has personal data that can be pulled out. The Office of General Counsel concurs that demographic data cannot be collected if a system of records is not available.

To set up a system of records, an agency must publish an announcement of the system in the *Federal Register*, inviting public comment. It must identify the government statute(s) that allow collection of such data and explain what data would be collected, who would see the data, what the data would be used for, and how the data would be protected.

The plan is to establish the Strategic Integrated Procurement Enterprise System (STRIPES) as a system of records into which grants.gov will enter all proposals and applications. STRIPES should go online in January 2008. All DOE procurement will go through this system. There are two options for SC data collection: using the personal-data form from grants.gov or establishing a separate stakeholder registration system that requires people to register prior to submitting proposals for review. With the latter option, personal data are entered into a separate section. Orbach selected this second option.

Grants.gov has a government-wide Research and Related Personal Data form; DOE does not use it; with DOE, the submission of personal data is voluntary.

If the first option were chosen, STRIPES would need to be made a system of records, additional data protection may need to be added to the SC central hard drive, and IMSC may need to be made a system of records. The second option is essentially the eRA Commons of the National Institutes of Health (NIH), which employs a credential (e.g., an agency login). DOE uses such a credential in certain applications.

If the second option were selected, information would go into a second, separate system. A new system of records would need to be created with a connection to the main system through a unique identification number.

Whichever option is selected, additional funds would be needed.

Hemminger stated that Ray Orbach is enthusiastic about moving forward with this project but wants it done SC-wide. Cummings noted that this is the same method used by the NIH.

Plummer asked how this system would track referees. Blevins replied that it tracks referees to some degree now. They could be asked to register in this system, and then it could track them by that personal information provided.

Richards asked how long it would take to set up this system. Blevins replied that she would have to ask the IT [information technology] people about this. DOE also needs to build on what the National Science Foundation (NSF) and NIH have done.

Hemminger turned the discussion to the BRN workshops. **John Sarrao** was asked to review the Workshop on Superconductivity.

World and domestic energy demand is increasing rapidly, producing a grand challenge for production, delivery, and use. The electricity grid, an essential energy backbone, is under stress for a number of reasons: (1) Demand is growing. (2) Reliability is less than required, with blackouts, cascades, and quality problems. (3) 7 to 10% of the power is lost in the grid, the equivalent of a 40-GW power plant.

SC can affect power production, delivery, and use. To see how, a Workshop on Superconductivity was held on May 8-11, 2006. It had panels on materials, phenomena, theory, and applications. The consensus of the workshop was that superconductors can transform the power grid to deliver abundant, reliable, high-quality power for the 21st century. Progress is going on today. The focus of the workshop was on performance, cost, and materials. In performance, an order of magnitude increase in current-carrying capacity and an order of magnitude reduction in alternating-current loss are being looked for.

Workshop participants identified seven priority research directions and two cross-cutting research domains. In materials, it is desired to make search and discovery for new superconductors more directed and to control the structure and properties of superconductors down to the atomic scale and maximize the current-carrying ability of superconductors with scalable fabrication techniques. To do this, one needs to understand and exploit competing electronic phases. Mechanisms also need to be studied to develop a comprehensive and predictive theory of superconductivity and superconductors and to identify the essential interactions that give rise to high-Tc superconductivity. The two cross-putting issues identified were (1) the need for new tools to integrate synthesis, characterization, and theory and (2) enabling materials for superconductor utilization at low temperatures.

Materials need to be translated from discovery to design. A plot of temperature versus time since Bednorz and Mueller’s breakthroughs in the 1980s shows that performance is increasing by design. The phase diagrams of today’s superconductors are much more complex than those of a few years ago. Not only a global knowledge but also a “mapping of the genome” of high Tc are needed; then one would not need to know *everything*. Most opportunities lie in non-cuprate materials (e.g., niobium).

In applied research, there are short-term milestones, but there are science challenges to be addressed that will drive progress forward (e.g., understanding atomic-scale control of materials’ structure and properties). Superconductivity spans all four columns of the four-column chart (discovery research, use-inspired basic research, applied research, and technology maturation and deployment) quite well.

Grand challenges in superconductivity are

- To transform the power grid to deliver abundant, reliable, high-quality power for the 21st century
- To discover the mechanisms of high-temperature superconductivity, going beyond the cuprates
- To shift from “materials by serendipity” to “materials by design”
- To be able to predict and control the electromagnetic behavior of superconductors from their microscopic vortex and pinning behavior

The world is on the verge of the 50th anniversary of BCS [Bardeen-Cooper-Schrieffer] Theory and the 20th anniversary of high-Tc cuprates. The discovery of MgB was serendipitous but has evolved quickly. There are underlying principles that drive the understanding of phase diagrams of new fields of complex materials: (1) quantum correlation techniques for other fields of science and (2) complex and collective phenomena. A large number of scientific techniques and capabilities were far less developed in 1987 than they are today and have benefited tremendously from cuprate-based superconductivity.

Superconductivity is an essential driver for materials discovery, insights into collective phenomena, and new tools and methods.

Plummer stated that the science of superconductivity is driven by serendipitous discoveries in materials science. Sarrao agreed.

Moskovits asked if anyone had looked at the world supply of yttrium and other rare elements. Sarrao acknowledged that there are nagging questions about the availability of these materials, but that cannot drive scientific research.

Isaacs asked if this was a network issue or something else. Sarrao replied that it was. The question comes down to, can you push more power through a cable?

Julia Phillips was asked to report on the Workshop on Solid-State Lighting held in May. The purpose of the workshop was to identify basic research needs and opportunities underlying light-emitting diodes (LEDs) and related technologies with a focus on new or emerging science challenges with the potential for significant long-term impact on energy-efficient and productivity-enhancing solid-state lighting (SSL).

Lighting is the largest fraction of energy consumption. About 20% of electricity consumption is for general illumination. Incandescent lighting is only about 5% efficient; fluorescent is 25%. With incandescent lighting, most energy is turned into heat. SSL is more efficient than incandescent lighting by a factor of 10, and more efficient than fluorescent lighting by a factor of 2. The goal is massive adoption of 50% efficient SSL, which could produce a reduction in electricity consumption thereby affecting electricity generating capacity and carbon emissions.

The workshop had three panels: LED science, organic light-emitting diode (OLED) science, and cross-cutting science. There were 79 participants from academia, national laboratories, federal agencies, industries, and foreign countries. The proof of potential has been the development of the JDS Uniphase (JDSU) IR laser with 76% efficiency. However, the state of the art of white-light LEDs is less than 10% efficiency. A high-efficiency white light needs to be developed.

The workshop panels were charged with developing priority research directions and grand challenges (crossing panel topics). The LED science panel focused on inorganic sheets, which have gotten a lot of attention but have a long way to go. The OLED science panel reviewed recent interests and discoveries. And the cross-cutting-science panel looked at emerging developments in nanoscience and controls.

One grand challenge was seen to be the rational design of SSL structures. Today, many layers are used, the interactions of which are not understood. Those interactions need to be understood. Optimum structures need to be predicted through multiscale theory and modeling, and fabrication of materials and structures needs to be designed to optimize the optical and transport properties. The physics needs to be understood, and the physical properties of both n-type and p-type materials need to be precisely tuned. In chemistry, high-quality materials need to be made, and high-precision placement needs to be developed. Finally, a theoretical understanding of structural effects is needed. New functionalities need to be developed through heterogeneous nanostructures, innovative photon management, enhanced light-matter interactions, precision nanoscale characterization, synthesis, and assembly; quantum applications to light extraction; and conventional light-emitting semiconductors; photon-conversion materials; and understanding degradation in OLEDs.

A second grand challenge is the control of radiative and nonradiative processes in light-emitting materials. The challenge here is to understand and control the physics of photon generation and emission and how to channel light out of the device. To do this, multiple fronts need to be attacked. Some of the science questions and opportunities are: What limits the electroluminescence efficiency of inorganic and organic semiconductor LEDs? What are the roles of extended and point defects, polarization fields, and material inhomogeneities? Can defects and nanostructures be tailored to achieve higher efficiencies? Can radiative rates be enhanced through the modulation of the photonic density of states (e.g., through photonic lattices)?

A map for deployment of SSL was developed. The workshop report will be available in the next few weeks.

Morse noted that SSL is the inverse of photovoltaics and asked whether SSL and photovoltaics can progress in tandem. Phillips replied that one of the plenary speakers alluded to such a synergy and that the allusion came up time and again in the workshop.

DiSalvo noted that increased efficiency has always led to increased use. Phillips responded that the sense is that electricity use can be flattened out and may actually be decreased.

Hemminger called for a break for lunch at 12:24 p.m.

Thursday, August 3, 2006
Afternoon Session

The meeting was called back into session at 1:30 p.m., and **Raymond Orbach** presented an update on the DOE science programs.

The Energy Policy Act of 2005 created a mandate for science and opened up new opportunities that are still being explored. It also facilitated the President’s ACI and Advanced Energy Initiative (AEI) in the FY07 budget request, calling for a 14% increase in the SC budget in FY07 and doubling it in the next 10 years. Both houses of Congress have largely supported the President’s request for FY07, showing Congress’s confidence in the scientific community. The House maintained funding for DOE SC at the President’s 2007 request level, and Congressionally directed funding is *above* the

President's request. The Senate Appropriations Committee reported the Senate Energy and Water Appropriations Bill to the floor. SC funding is at the President's 2007 request level, but no date has been set for a floor vote, and that might not occur until after the election, requiring a continuing resolution, possibly deferring the 14% increase in funding.

The Department is thankful for the Presidents request and Congress's support of it. The SNS was commissioned on schedule, slightly under budget, and with increased scope. There are major new initiatives in the FY07 budget, including the LCLS-II (the second phase of the Linac Coherent Light Source).

Section 1006 of the Energy Policy Act creates the position of Under Secretary of Energy for Science with a withering list of responsibilities, which extends to applied programs and to National Nuclear Security Administration (NNSA) programs. That position now has responsibility for science at all of the national laboratories.

On July 3, Secretary Bodman stated that, "the primary responsibility of the Under Secretary for Science is to advance the science portfolio at the Department of Energy and to strengthen the contributions of science to all of the Department's activities in collaboration with the Under Secretary and the Under Secretary for Nuclear Security." This is a mandate to work with all the applied programs. It is imperative that SC be at the leading edge of science and technology. And the applied areas have to be in touch with quality science. Conducting applied research in an effective manner is being encouraged. Those applied programs are not being taken over; their risks are being mitigated. A brain trust is being put together to serve both discovery science and the applied-science program, including stockpile stewardship and nonproliferation. Stewardship and the scientific community should be indistinguishable, as in the National Ignition Facility. Workshops will be held to engage the scientific and applied-science communities. The first workshop has already been held on superconductivity. Industry has already picked up on results of that workshop. The day before the present meeting, the first Global Nuclear Energy Partnership (GNEP) workshop was held; it will produce a series of related workshops. The Under Secretary for Science will continue to be the Director of SC in the next couple of years.

The day before this meeting, the startup of two bioenergy research centers was announced. They are to study solar-to-fuel and the tuning of the genomics of fuel sources to enzymatic appetites. The risk is so high that the private sector is not pushing this research; but the payoff is so high that the government has a responsibility to look at it. $25 million is going to be devoted to these two centers to explore metabolic pathways.

SC has worked on the hydrogen issue and on materials closely with the Office of Energy Efficiency and Renewable Energy (EERE) and with the Office of Advanced Scientific Computing Research (ASCR) on high-performance computing and carbon sequestration. The mathematics are the same for the vadose zone at Hanford, Yucca Mountain, and carbon sequestration. Stability of the electricity grid is a control problem, and the applied-science programs can provide SC a lot of experimental opportunities.

Hemminger asked if the Office of High Energy Density Science (HEDS) is to be in SC. Orbach replied that the establishment of that office is directed in the Senate mark to be in the purview of the Under Secretary for Science. The Under Secretary's office is still in the midst of responding to that mark. HEDS is an area that has not been addressed well. One approach is to use an interagency task force (IATF) to develop a roadmap for the pursuit of this science. A report from that IATF is expected in December.

Moskovits asked if the mandate of the cellulosic biofuels center would include other types of chemistry that cellulose does not normally see or if it would be biologically focused. Orbach replied that the funding-opportunity announcement was purposely quite broad. It is desired to be as flexible as possible. Somehow, termites turn cellulose into energy. People need to find out how to do that same task. It may also be desirable to modify the cellulose. An investment here could have profound results.

Greene stated that bridges between industry and science are needed. She asked how the International Thermonuclear Experimental Reactor (ITER) is progressing. Orbach answered that the site has been selected. Working with international colleagues is very difficult. There are six deputy director generals. The Director and Principal Deputy Director are from Japan and the EU, respectively. One now needs to get ITER to work. The international agreement is now before Congress. The organization cannot be stood up until all seven parties ratify the agreement, perhaps a year from now. The Department is working very hard to make it work.

Hemminger commented that it is important to recognize the great value of SC for basic science; it is not just a job shop for solving problems for applied science. BESAC's subcommittees will provide advice on how to preserve this basic role while cooperating with the applied sciences.

Morse stated that a lot of research at universities is appearing on the restricted list. Orbach replied that the Department of Commerce is dealing with this issue well; it is a very sensitive issue. The ability to do basic research should be protected. Morse specifically pointed to the fact that the limit on photovoltaic research has been made more restrictive. Orbach answered that the system seems to be working well, and it is hoped that it will address and resolve that problem.

John Miller, **James Roberto**, and **Tomas Diaz de la Rubia** were asked to report on the Workshop on Advanced Nuclear Energy Systems.

The workshop had 235 attendees. A "technology perspectives" document was distributed to all panelists one month in advance of the workshop. A plenary session was held on the first day on the (1) technology perspective, (2) industrial perspective, (3) international perspective, and (4) science frontiers. Breakout panels were held on technology challenges, current status of research, basic research challenges, opportunities, and needs; priority research directions; relationships between science and technology; and cross-cutting research. The full workshop report will be issued within the next eight weeks.

Eight needs were found:

- A radical improvement in the fundamental basis for developing and predicting the behavior of advanced nuclear energy systems
- A predictive, simulation-based method to shorten development and qualification times for new fuels and materials and to facilitate the design of safer and more-efficient nuclear energy systems
- Advanced structural materials that can withstand higher temperatures, higher radiation fields, and harsher chemical environments

- Flexible and optimized separation and reprocessing schemes that will accommodate the varying radiation fields produced by waste streams and input feeds
- Avoiding separated plutonium and achieving improved yield and separation factors
- New and novel waste-form materials tailored to a wide range of waste-stream compositions from advanced fuel-cycle technologies
- Long-term prediction of waste-form performance in coupled, complex, natural systems
- Proliferation resistance through physical protection and material accountability with improved precision in materials accountability for industrial-scale separation plants, including sampling methods and detectors

Current theory and simulation methods are inadequate to address complex, multicomponent systems in extreme radiation environments, especially for actinide materials. Failure and corrosion mechanisms in chemical and radiation environments are poorly understood. There is a need to understand the full chemical and physical phenomena in multicomponent systems from femtoseconds to millennia at temperatures of 1000° C or more and to radiation doses to hundreds of disintegrations per annum. To do this, the emergence of ultrafast experimental probes needs to be taken advantage of. Materials need to be manipulated at the nanoscale to tailor new functionalities in extreme conditions. The greatest opportunity lies in establishing a science base that enables one to move away from lengthy and costly empirical approaches to fuel development and qualification. The greatest challenge is to understand and predict the broad range of nuclear, chemical, and thermomechanical phenomena that synergistically interact to dictate fuel behavior.

This workshop was asked to identify research directions, going from scientific challenges to research direction to potential scientific impact to potential impact on advanced nuclear energy systems. It was then asked to put together a map of the relationships between the science and the technology. From that process, the workshop produced 25 such charts, which were then compressed to 9. Two of the priority research directions were:

- Radically extend the radiation-resistant properties of materials and interfaces and extend performance limits for structural applications, tools, and waste forms.
- Develop predictive multiscale models for materials and chemical phenomena in multicomponent systems under extreme conditions.

Cross-cutting themes were

- Strongly coupled, multiscale experimental and computational studies
- The exploitation of DOE tools to investigate nanoscale structure/dynamic and ultrafast experiments
- New approaches for enabling access to forefront tools
- Assessment of workforce issues in nuclear-related research
- Safety and nonproliferation opportunities

A map of the relationships between the science and technology was developed for the whole workshop; it constituted a first cut in mapping out a research agenda.

Hemminger thanked the SC staff and workshop managers for putting together such a productive meeting.

Moskovits noted that not many universities are working in this field of nuclear power. Roberto agreed that that is true, and there will probably be a recommendation on that topic.

McCurdy stated that the understanding of electronic structure is pretty ad hoc. New theories are needed, and they require experiments. He asked if the workshop discussed the need for theory. Diaz de la Rubia replied, yes, especially in the cross-cutting panel. Each of the other panels also recognized the need for theory. McCurdy asked if there were practical barriers to doing these experiments. Diaz de la Rubia responded that there are barriers but nothing fundamental.

Gates asked how the list would have been different 10 years ago. Roberto answered that what is new are capabilities, especially on the experimental and computational sides. This field needs to understand how to employ those new capabilities. Kohn added that the playground has, indeed, changed; plus there is a daunting energy crisis. Because of the difficulty of working under extreme conditions, one needs to use theory, simulation, and modeling. These problems are so complex, theory will have to advance by using experimentation at every stage.

Cummings asked how much of the Accelerated Strategic Computing Initiative (ASCI) program rolled over into this effort. Diaz de la Rubia said that some aspects of ASCI contribute to this program. There is a clear synergy between the two areas of investigation.

George Crabtree was asked to report on the Laboratory Working Group (LWG) assessment of DOE's energy portfolio.

In his Senate confirmation hearing as Under Secretary for Energy and Science, David Garman said "we have not done as good a job as we should in coordinating the activities of the ESE [Energy, Science, and Environment] offices. We have not done as good a job as we should in performing the cross-cutting analysis to justify our budgets to the Congress." There are now two under secretaries, one for energy and one for science. Reporting to them is an R&D Council that has an internal working group and national laboratory working groups that draw upon the expertise of analysts.

In the FY05 appropriation, energy was allotted \$2.5 billion, science was allotted \$3 billion, and environment was allotted \$7.8 billion. In addition, the applied-energy R&D portfolio was allotted \$1.4 billion, which went to energy efficiency and renewable energy, fossil energy, nuclear energy, and electricity delivery and energy reliability.

The charge to the laboratory working group was (1) to deliver improved analysis and decision support material to senior management for the FY08 budget process with an emphasis on simplicity, timeliness, clarity, and relevance; a focus on impacts and risks; and drawing on the best available knowledge and (2) to develop a sustainable long-term portfolio-analysis capability and process that is credible; incorporates technical, market, and other risks; and enables a timely response. This is an enduring multi-year process.

The National Energy Policy has four broad goals to be advanced:

- To diversify the energy mix and reduce dependence on foreign petroleum, thereby reducing vulnerability to disruption and increasing the flexibility of the market to meet U.S. needs.
- To reduce greenhouse-gas emissions and other environmental impacts from energy production and use.

- To create a more flexible, more reliable, and higher-capacity U.S. energy infrastructure (electricity grid), thereby improving energy services throughout the economy, enabling use of diverse sources and improving robustness against disruption.
- To improve the energy productivity of the U.S. economy.

The LWG highlighted six conclusions: the highest-leverage approach to reducing petroleum imports lies in transportation fuel-switching and efficiency improvements. For the near term, this includes clean diesel, hybrids, and ethanol; for the long term, it includes cellulosic ethanol, fuel cells, and energy storage. Material reductions in carbon emissions depend on progress in zero-net-emission electricity generation options and fuel switching accompanied by efficiency improvements throughout the economy. In the near term, this includes building technology, hybrid electric drives, biofuels, advanced nuclear, and zero-emission fossil fuels; for the long term, it involves utility-scale solar, bio-energy feedstocks, and biomimetic energy conversion.

Several areas of science offer great promise for advances that could transform energy technology. For example, design and synthesis of materials exploiting nanoscale understanding, predictive modeling of complex systems, and scattering facilities for in situ molecular characterization.

Two areas of science may merit consideration for increased attention within the portfolio: systems and synthetic biology and the catalysis and separation of chemical transformations.

There are two significant gaps in the portfolio that may retard progress toward national goals: (1) carbon dioxide sequestration science and technology (DOE is not doing enough in this area) and (2) next-generation electricity-grid technologies.

Refining R&D portfolio management practices could accelerate progress and create a pipeline of innovations targeted on national priorities. DOE should focus on defining critical outcomes to impact national goals, strengthen horizontal and cross-cutting integration, align research strategies from discovery to technology deployment, and consider use-inspired science initiatives to drive breakthrough discoveries into applications.

The transportation sector would benefit from fuel switching to ethanol-from-sugar, biodiesel, oil shales, coal liquefaction, enhanced oil recovery, heavy-crude processing, and auxiliary power options and from higher efficiencies in propulsion and vehicular systems. The electricity grid would benefit from switching to nuclear, zero-emission fossil fuels, and renewable energy; by upgrading to a more-reliable and secure system; and by increasing electricity-use efficiency through zero-energy buildings, solid-state lighting, and efficient processing.

One gap that DOE faces is translating basic research to targeted R&D; another is translating nearly mature technologies from working prototypes to commercial deployment. Both of these are bidirectional issues.

The next issues the LWG should consider include the interaction of fuel sources in fuel switching, including tradeoffs among coal, gas, nuclear, and renewable for producing electricity and among petroleum, biofuels, and alternatives like hydrogen for transportation. It should also consider the interaction of energy chains and develop tools for the quantitative analysis of energy systems (looking at market inertia and ripple effects across sources and chains).

The LWG should also analyze the potential of science for energy solutions. Science should be looking for revolutionary (order-of-magnitude) breakthroughs, not evolutionary (10%) increments. New approaches are needed for managing the basic-applied interface; these two activities need to establish a greater synergy while maintaining their separate identities. Discovery science needs to be emphasized as distinct from use-inspired basic research (the latter has caught on well). The frontier (small, fast, complex, etc.) needs to be advanced; the new knowledge will lead to unexpected new uses. To do that effectively, one needs to understand the grand challenges of discovery science.

A break was declared at 3:21 p.m., and the meeting was reconvened at 3:47 p.m. Hemminger commented on the fact that the success of the workshops in bringing in new funds has shrunk the core research portfolio. The Committee should not neglect its responsibility for nurturing that core research and grand-challenge science. The process of coming up with brilliant ideas is difficult. BESAC will continue these workshops for some time in the future.

Graham Fleming reported on the Subcommittee to Investigate Scientific Grand Challenges. The question before that Subcommittee is whether there are schemes that, if successfully implemented, would produce breakthroughs leading science into new areas. The Subcommittee seeks to create a set of about 10 grand challenges that define the discovery-science portfolio of BES. It includes representatives from industry, national laboratories, and universities.

This area has been extensively worked over, including in a new report from the National Research Council (NRC), *Controlling the Quantum World*. Preliminary questions were developed by BESAC at an earlier meeting. The challenges were defined by circulating a questionnaire that asked, what is your big question?

The first meeting of the Subcommittee was held in Berkeley on June 26-27, 2006. Each member brought 1 to 22 big questions, such as:

- What are the limits of energy conversion?
- How is the lowest energy pathway sought?
- Can atom-efficient catalysts selectively transform matter?
- Can atomic imaging be extended to molecular movies?

The big question is, can one understand and predict how cooperative phenomena emerge from ensembles of simple components rather than degenerate into chaos? The challenge is to understand, measure, and use materials and processes in unusual and extreme environments.

Five new topics were identified:

- Creating a new language for electronic structure by defining the real-time dynamics of electrons in atoms and molecules
- Defining cardinal principles of behavior, describing the science of matter beyond equilibrium
- Understanding the basic architecture of nature, allowing one to direct the assembly, structure, and behavior of matter
- Discerning primary patterns in multiparticle phenomena explicating emergent, strongly correlated and complex systems
- Producing nanoscale communication

What does creating a new language for electronic structure mean? It means, how and why does the adiabatic separation of electrons and nuclei fail utterly? What are the manifestations in photodynamics? How does one measure it? How do electrons actually move in atoms and in molecules? Can one watch electrons and bonds? How does atomic and molecular matter respond to very short (attosecond) and very strong (terawatt) excitation? Can one control the motions of the interatomic electrons, driving processes in a desired direction?

The Subcommittee's views on the meaning of "a new language for electronic structure" included (1) the dynamics of interacting finite-mass nuclei and electrons, far outside the Born-Oppenheimer approximation, caused by high-energy and high-frequency incident radiation and particles; (2) what electrons are doing in molecules; (3) attosecond imaging for electronic intramolecular dynamics; (4) coherently controlled matter at ever increasing energy scales; (5) an ultrafast, coherent X-ray laser user facility supporting a large number of users; and (6) transition states in chemical reactions to create novel materials.

The cardinal principles of behavior are: When is a steady state attained? How do its properties differ from equilibrated states? How is structure determined away from equilibrium? Can one characterize and understand metastability? Can one design metastable structures for specific properties and applications? Are there variational principles, or thermodynamic laws, out of equilibrium? Can metastable structures be advantageous in sustainable processes? There is no equilibrium at the nanoscale, just transitions between metastates. An anticipated key benefit of a theory of organization and dynamics of matter beyond equilibrium would be fundamental design rules for classical or quantum machines of arbitrary size and operating arbitrarily far from equilibrium.

The basic architecture of nature refers to: How does the environment of a system modify and control its properties? How do structures behave under extreme environments (ultrahigh pressure and shock waves, extreme radiation, plasmas, etc.)? What are the nature and the limits of self-assembly? Can we create complex functional materials that can be fully disassembled and re-assembled? Can we design and build self-regulating, self-repairing molecular devices? Algorithms are needed for truly robust soft matter. Can key energy-transducing biological devices be connected to nonbiological devices?

In regard to emergent, strongly correlated, and complex systems, the Subcommittee talked about expanding chemistry from considering the properties of pure substances to considering the properties of organized multimolecular interacting systems. It also asked whether one can use quantum molecular dynamics to predict thermodynamic pathways at the atomic scale.

In nanoscale communication, it was asked if one can wire up the biological world for energy and information transfer and whether one can build devices that fully integrate living and nonliving components. One can improve the thermodynamic efficiency of computing machines by six orders of magnitude or more while at the same time substantially increasing the computational throughput by three or more orders of magnitude. These pieces need to be stitched together.

The Subcommittee has to determine the domain in which these questions operate. At its next meeting on Aug. 4-5, after the BESAC meeting, the Subcommittee will refine and focus the challenges, identify and recruit expertise from outside the Subcommittee, explore mechanisms to engage a broader community, and establish a timeline.

Clark said that a major problem is that many problems are framed in multiple scales; one such scale is the temporal. In such cases, one may have many small time scales and need to consider long time scales, as well. Fleming agreed.

Johnson asked what Dehmer’s reactions were to the first discussions. Dehmer replied that the topics related to users’ needs rather than to discovery science.

Hemminger added that the Subcommittee had to grapple with the question, How do you do anything other than a laundry list of exciting topics? It has to bring out the underlying fundamental science questions.

Flynn pointed out that changes in technology open up new opportunities to address questions that have been around a long time.

Plummer said that he would like a grand challenge on observing and measuring nanoscale events in real time. Fleming replied that he would like to achieve some focus before letting the technologists lead the science.

Ceyer said that diatoms and molecules would answer a lot of questions. That would be a grand challenge. Ratner responded that that is the first premise of the Subcommittee. It would like to know if the five directions chosen are the right ones.

Moskovits stated that, ultimately, this is about money. Where in our best work is the best investment? Is there an incremental increase that would produce a non-incremental reward? Is there something in this exercise that would not have happened anyway? Fleming said that that is why timing is important. The Subcommittee has to have some inkling on how to proceed.

McCurdy pointed out that technology follows science after a long time lag, but science follows technology with almost zero time lag. Timing needs to come across clearly in the report. The basic questions are still not coming across and becoming understandable and obvious. There are now a lot of little questions out of which the Subcommittee is trying to make a big question. He was surprised that the question of whether quantum communication can become technology did not come up.

Hemminger passed out questionnaires for Committee members to fill out for discussion the next day.

Cummings suggested making a list of what one does in each of the five areas. These should be described at a high-enough level but still be understandable by nonspecialists.

Morse stated that these questions range from the profound to the technologically cute and asked what the unique fundamental enabling mechanisms are and whether those capabilities can be captured. What is the fundamental nature of matter and energy? Fleming said that he fully accepted all of those comments.

Gates noted that most of the questions are inspired by nature and biology. He would look for imagination and asked rhetorically whether anything gets inspired from lists like this. Fleming suggested that the world could always wait for another Einstein to come along. Hemminger pointed out that this project has several goals: Inspiration and articulation of important science to design matter.

Wirth suggested not saying what should be done but what one will get out of it. The final report should be one that Congress can understand, stating what the problems are in learning these things. Hemminger cautioned that one does not want to get ahead of oneself. First, the exercise needs to be done, and then the report needs to be written.

DiSalvo noted that *Quarks to the Cosmos* posed questions but no statement of economic benefit, and Congress and OMB got excited about it.

McCurdy asked why they were so successful and BESAC cannot articulate the basic questions. Their questions are stated simply (e.g., what is dark energy?). Pulling out the basic question is a different intellectual exercise. BESAC tends to deal with many, many details. Ratner stated that that is exactly right. We know too much. It sounds like some of the five questions are the right ones, and some are not.

Hemminger suggested thinking about the problem overnight. The hard part, coming up with the questions, has not been addressed yet. Rather, the Committee has addressed how to communicate to the nonscientific community. The Subcommittee needs to move ahead. Now is the time to formulate the questions to be addressed. There will be time later to talk about the audience and message formulation.

Isaacs objected that one needs to know the target audience. Dehmer stated that this conversation was held 5 years ago. Sometimes one does not know the audience. Concentrate on the first three questions and ignore the questions on funding.

Hemminger called for public comment.

Michalske suggested that the Subcommittee may want to identify previous grand challenges that have substantially changed.

The meeting was adjourned for the day at 5:00 p.m.

Friday, August 4, 2006
Morning Session

Chairman Hemminger called the meeting to order at 8:44 a.m. He welcomed the members of the Subcommittee to Investigate Scientific Grand Challenges to the table. He ordered people to turn in their “homework” and asked Dehmer to summarize the state of the discussion.

She noted that two-thirds of the original questions submitted to the Subcommittee were on the topic of sustainability, a term that is politically charged. The buzzword for this administration is economic competitiveness. The four broad national energy policy goals are

- Diversify our energy mix and reduce dependence on foreign petroleum;
- Reduce greenhouse-gas emissions and other environmental impacts;
- Create a more flexible, more reliable, and higher capacity U.S. energy infrastructure; and
- Improve energy productivity.

This is what one might call sustainability, but couched in national-policy terms.

Kohn noted that BESAC is a science group and often does not draw the distinction between science and policy. But science should affect policy. This administration withdrew from the Kyoto Protocol because of economic impact and scientific inconclusiveness. How science is conceived, presented, and used to influence policy is important.

Ratner asked for help for the Subcommittee. He introduced the members of the Subcommittee present. He cited three crucial concepts: (1) The fifth column on the four-column chart, which should define the fundamental science for the portfolio. (2) The list of members. (3) Grouping these many, specific topics by clear overarching questions about fundamental science. The five new topics introduced the previous day were modified overnight:

1. How do electrons and nuclei look in real time?
2. Are there general principles of nonequilibrium behavior?
3. Do we design materials randomly or rationally?
4. Where is the average behavior not good enough?
5. How do we interrogate and communicate with the unique world of the nanoscale?

The Subcommittee members now need to act as scribes for the suggestions of the Committee.

Kohn offered that the first question does not look exciting. This a grand challenge because there are situations where it is necessary to understand this in the regimes being produced by high-frequency, high-intensity, high-energy machines. It needs to be made obvious why this is a grand challenge. Ratner noted that the Subcommittee would like to refine these questions with subtitles and subquestions. Kohn said that the grand challenge is to develop an approach that explains why current systems fail. Ratner agreed that a meaningful and powerful expression is needed.

Cummings suggested, “Can we see electrons and nuclei?”

Spence noted that there is a proposal to experimentally “see” molecules in movies of diffraction patterns.

Isaacs suggested, “What is the nature of the chemical/physical bond?” Scanning transmission electron microscope (STEM) and scanning tunneling microscope (STM) images show not only atoms but also the stuff between. This needs to be put it in terms that are compelling.

Richards stated that the third question leaves out directed assembly and loses the romance of connecting to nature.

DiSalvo suggested, “Why do electrons in some materials behave in complex ways?” with the grand-challenge subcontext: “What new behaviors lurk in such systems? How do we find and explain such materials in a timely manner?” These questions are related to the first, third, and fourth questions and maybe to the second.

Hemminger observed that the homework assignment was to come back with missing grand-challenge questions, not to wordsmith. Intellectual input is needed.

Moskovits stated that a focus is missing. The frontier has to be pushed. The connection between science goals and technology has to be made obvious. The marriage of biology and technology should be highlighted. “How much of the biomachinery of the cell can be replaced by technology?” These statements, as presented, do not speak to a broad-enough audience. Morse agreed that they need to be galvanized.

Hemminger suggested that a useful grand challenge might be the invention of experiments that cannot be done yet (e.g., imaging electrons at all time scales without their sitting on a surface).

Wirth said that if the portfolio is to be re-diagnolized, the current portfolio needs to be looked at, and the barriers it faces need to be identified. Those are the challenges.

Miller suggested being careful about using words (like bio-inspired molecules) that have other meanings. BES would like to be inspired to fill out the portfolio as it *should* be.

McCurdy said that the Committee was not getting off the ground because each of the five questions requires one to be a specialist. No wordsmithing will overcome this problem. The technological problems are understandable. Things should be organized differently.

Ratner stated that Congress and the *Washington Post* are two targets, but scientific colleagues are another.

Hemminger disagreed with McCurdy. There is a very good mechanism in place to identify science challenges: the BRN workshops. They have been very successful and have led to budget increases, although the core research has decreased. The technologically independent, fundamental science questions need to be identified. That is a difficult task.

Kung stated that it is important that this report give a really forward-looking position. The first question just reflects one part of the question but misses condensed matter and many other crucial issues. In the second question, the difference between ground state and excited states is important but overlooked. The third question begs the question of the organizational principles that govern behavior. We would like to see the whole core research portfolio represented. Such questions as, "What are the origins of material strength?" need to be addressed. Ratner responded that, to express such issues as succinct grand challenges is very difficult. The scientific community is trying to develop an understanding of a huge number of phenomena. The Subcommittee will struggle to get the points put forward into the final list.

Gates suggested that perhaps several kinds of lists should be gathered to be mapped into the final list of grand challenges. The Subcommittee is trying to get the right words; it should read Gary Larson cartoons to find the right words to connect to the key audience.

Taylor noted that the same problem was faced by the hydrogen report: finding the right beginning of the report rather than the details that follow. One also needs to seek out *long-term* goals.

Greene stated that scientists do not know how to get their language across. They should read the paper Hilbert wrote in 1900 about the course of math in the following 100 years and David Gross's 25 questions in business for the next millennium. Ratner cautioned that Hilbert energized mathematicians but not the ordinary newspaper reader.

Odom noted that there are good fundamental questions underlying all of the problems faced. A lot of these are fundamental concepts that can be captured.

Wirth stated that scientists do not care about common people's understanding of science. The world is facing the economic development of China and global warming. If this report starts by talking about electrons, the general reader will not get it.

Spence said that, if one runs power plants at higher temperatures, one gets better efficiency and thus lower fuel use and CO_2 production. The development of materials that would make that possible would be important and comprehendible.

McCurdy wondered if the mission of BES is comprehensible; not if we talk about electrons, but yes if one puts it in terms of power production. Even among specialists, the questions offered are not understandable and doomed to failure. Instead, one needs questions such as, "Can you link all time scales in manipulating matter?" Otherwise it is too difficult to make these questions comprehensible. Mastering matter is an underlying goal.

Richards urged the Committee to get it right and *then* get it written. The Subcommittee needs to get the science right then months from now get it written properly. Trying to do both at the same time is futile.

Marks agreed. This will go through many iterations.

Wirth objected that what was going on was not trying to get the right language. Energy is a huge societal issue. This report needs to talk about more than the science.

Berrah added that one needs to relate to societal needs: new sources of energy and better standards of living. Biophysics is very important; science needs to be pushed in order to cure diseases. So the questions become: How do we get cheap energy? How do we cure diseases? The questions have to frame the big picture and let the subsections tell how the answers can be approached.

Kohn pointed out that Dehmer had shared a table with four columns. The first column was discovery science, then user-inspired science. That column should be kept in mind. It enables one to better communicate to the general public. It tells one what *use* the science is. Dehmer agreed. If one can choose the right big question, the connections will flow from one column to the next. But to go in the other direction is very difficult.

A break was declared at 10:23 a.m., and the meeting was reconvened at 10:48 a.m. Hemminger stated that the Subcommittee has to do the major work on this project. This meeting is an opportunity for the Subcommittee to get BESAC's ideas about science. One needs to focus on scientific topics.

Plummer pointed out that technology does things that nature never does. That is the challenge: to expedite discovery. Humanity does a terrible job of it now. No one is working on new materials.

Richards said, one cell, one molecule.

Marks asked rhetorically what was meant by grand challenge: something that violates current paradigms, which, if discovered, would have great impact. Each question will have several sub-bullets that address the interests of biologists, chemists, physicists, etc.

Phillips asked if the Subcommittee's perspectives are to be limited by what can be imagined today.

Greene stated that some of the current questions cover everything from seconds after the big bang to superconductivity. The beauty of science itself has to be in there.

Moskovits said that this report has to be about science, not technology. Technology has to be in there, but the science has to lead. The right type of things has been captured, but what Kung mentioned has to be captured, also. But the words selected aren't working; the words need to be crafted to be understandable in the same way to all readers. He was happy with the gist of the five questions. Everything fits under them. Everyone understands the concept of "striving." One doesn't need to draw the map, simply state the striving for the smallest, coldest, most energetic, or whatever.

Ceyer said that the Subcommittee has to express the basics of each question and then flesh each out out so each member of the scientific community understands it from his or her own perspective.

Johnson offered that the tools lead the science.

DiSalvo pointed out that the Subcommittee is not limited to five grand challenges. The brainstorming should not be limited. Each "take" should be explored. The writing will be good if the font-end assessment of science is good.

Cummings said that nonequilibrium systems have been investigated and experimentally verified. There are quantum versions of it. That is not as much a grand challenge as the others are. One can be too specific about these grand challenges. They need to be formulated at a high level. Gates added that the Subcommittee should get as long a list of candidates as they can and then winnow them down. A science writer should have been a part of the Subcommittee.

Kohn was unclear about the two lists. Ratner said that one was the one from the previous day, and one was the one from the current day. Kohn asked what the fourth question meant. Ratner said, the emergent behavior of complex behavior. He suggested that it come off the list. Kohn said that so many things come to mind; there are some good selections and some bad selections. An important aspect is timeliness. What questions are arising *now* or are particularly important *now*? Should timeliness be a criterion in selecting these grand challenges? Graham replied, yes; there has to be a connection to progress being made on a 10- to 20-year time scale.

Cummings pointed out that nowhere in these questions is energy mentioned. Miller explained that the mission needs are covered in the Basic Research Needs workshops. What is needed here is inspiration for the core research program. Ratner asked if the word energy needed to appear. Dehmer replied, no.

Hemminger encouraged the Committee members to stay in contact with the Subcommittee. He asked for public comment. There was none. One of the next charges to the Committee will be a COV to the Facilities Division; he asked for volunteers for that COV. The meeting was adjourned at 11:23 a.m.