Minutes for the
Basic Energy Sciences Advisory Committee Meeting
August 10–11, 1999, Gaithersburg Marriott Washingtonian Center
Gaithersburg, Maryland

BESAC members present:

- David D. Awschalom
- Collin L. Broholm
- Jack E. Crow
- D. Wayne Goodman
- Jan F. Herbst
- Anthony M. Johnson
- Marsha I. Lester
- Anne M. Mayes
- C. William McCurdy, Jr.
- Franklin M. Orr, Jr., Vice Chair
- Geraldine L. Richmond, Chair
- Zhi-Xun Shen
- Sunil Sinha
- Joachim Stohr
- Samuel I. Stupp

BESAC members absent:

- Boris W. Batterman
- Patricia M. Dove
- James A. Dumesic
- Robert B. Horsch
- Linda Horton
- Walter Kohn
- Stephen R. Leone
- Richard E. Smalley
- Patricia A. Thiel
- David E. Tirrell
- Edel Wasserman

Also present:

- Paul Alivasatos, Department of Chemistry, University of California at Berkeley
- Anthony K. Cheetham, Materials and Chemistry Department, University of California at Santa Barbara
- Daniel S. Chemla, Director, Advanced Light Source, Lawrence Berkeley National Laboratory
- Patricia Dehmer, Associate Director, Office of Science, OBES
- Martha Krebs, Director, Office of Science (Tuesday only)
- Douglas Lowndes, Semiconductor Physics Group Leader, Oak Ridge National Laboratory
- David Moncton, Executive Director, Spallation Neutron Source Project
- William E. Nay, Security Management Team, Office of Science
- Charles V. Shank, Director, Lawrence Berkeley National Laboratory
- John Stringer, Executive Technical Fellow, Electric Power Research Institute
- Iran L. Thomas, Director, Division of Materials Science, OBES
- Peter G. Wolynes, Molecular Biophysics Training Program, University of Illinois

In addition, about 50 others were in attendance as observers.

Chairwoman **Geraldine Richmond** called the meeting to order at 8:21 a.m. and asked each panel member to introduce himself or herself. She then reviewed the agenda and introduced **Martha Krebs** to present an update on the Office of Science (SC): its strategic plan, R&D portfolio, new field management structure, and challenges and charges to the Department [including a new charge letter to the Basic Energy Sciences Advisory Committee (BESAC)].

The strategic plan cites five major goals: (1) to provide fuel for the future, (2) to protect our living planet, (3) to explore energy and matter, (4) to provide extraordinary tools for extraordinary science, and (5) to manage as stewards of the public trust. These goals reach across all SC organizations. The portfolio tracks FY 1999 and 2000 budget elements and will be available on the SC web page in September. Within this portfolio, the line items in the budget link to the goals of the Office and the Department. The plan resulted from a broad involvement with our community [laboratories, Congress, Office of Management and Budget (OMB), and the Office of Science and Technology Policy (OSTP)]; it is not just a top-down exercise. These documents convey to the rest of the Department, Congress, the laboratories and contractors, and the general scientific community an awareness of what SC and DOE do.

She reviewed the status of the FY 2000 budget and pointed out some highlights:

- the increase in BES's requested budget reflects largely the inclusion of construction costs for the Spallation Neutron Source (SNS);
- the Department asked $214 million for the SNS, the House markup contains $68 million, and the Senate markup contains $187;
- fusion energy's budget has held steady at the FY 1999 level, and the House has actually added about $28 million; and
- the request for computational technology research was $40 million more than last year's appropriation, but the House has reduced that request by $53 million and the Senate by almost $70 million.

The House and Senate markups provide funding that is a little better than flat from FY 1999. The National Science Foundation (NSF) and National Aeronautics and Space Administration (NASA) have been more harshly treated.

The appointment of Dave Moncton made a tremendous difference to the treatment of the SNS. The SNS review held recently affirmed the general approach, although it expressed lingering concerns about project management. The House is positive about the outcome of that review, and she anticipated an improvement in the House's funding that will make it closer to the Senate's level.

The FY 1999 appropriation of the Strategic Simulation Initiative (SSI) is $15 million above what was recommended by the Energy and Water Subcommittee. That complicates what goes on this year. The House left in the money for the next-generation Internet, but took away the authority; the Senate took away the funding. Other departments got mixed levels of funding for this initiative, but NSF did not get the money that was taken out of the Department of Energy (DOE) budget. Thus, under the current House and Senate markups, the next-generation Internet infrastructure will not be developed. However, in September, this topic will be a high priority of the administration, and it is possible that these funds will be put back into the budget.

The House markup includes a $43 million general reduction that will hit Defense Programs (DP), travel costs, environmental management, and laboratory-directed R&D ($30 million of the $43 million). This decision cuts to the stewardship of the laboratories.

On the topic of changes in management, she noted that the Secretary reconfigured the organization chart to emphasize more clearly the role of program offices. The staff and support have been shifted aside, and DP no longer reports to two managers. The field offices now report to specific program offices of the Department. A field-management council was established so that if the field offices want to establish a policy, they clear it go through the Council under the sponsorship of the program offices they serve. The field offices now report to the program offices of the four major business lines of the Department [DP, SC, Environmental Management (EM), and other programs]. The program-office responsibilities align well with the funding received by the field offices except at Oak Ridge, where a diverse mix of EM, Nuclear Energy Research (NE), DP, and SC operations occur. SC incorporates three of these field offices (Oakland, Oak Ridge, and Chicago). SC's budget and effort have always been focused on disciplinary stewardship. Now it will need to focus also on its performance in terms of the goals that have been identified.

The SNS and other programs have opened up opportunities for the different offices of DOE to work together and to make clear the needs for funding, where the funding goes, and where it is spent. The Department has also developed a good collaboration with the NSF to make obvious the needs for several multiagency programs and projects.

The new BESAC charge letter includes two charges to the Committee. It asks BESAC to review the Advanced Light Source (ALS) to develop a vision for the future and an assessment of

- the quality and diversity of the science programs to be conducted there,
- the user demand expected, and
- the interactions and relationships within the user community and between the user community and DOE.

The charge letter also asks BESAC to establish a committee of visitors to assess matters pertaining to program decisions and to review program management every three to four years. The first committee of visitors should be established by the year 2000. This approach to understanding how well the Department is doing would contribute to that gained by the GPRA (Government Performance Review Act) process.

Jan Herbst asked what the "Program Direction" line item is. Krebs replied that it paid for the Office's manager, assistant managers, and support services. Herbst noted that there was a $70 million difference between the House and Senate versions of the budget. Krebs said that that discrepancy arose because in the FY 1999 budget, money was moved around for reorganization of the field offices, education, and other programs, so there is some confusion about what should be taken into account in the FY 2000 budget.

Wayne Goodman asked about the directors' discretionary funding. Krebs said that the rules are that the laboratory directors cannot use these funds to augment activities already funded. The argument was put forward that that money was not made available for appropriated purposes, and

Congress saw these dollars as being the use of taxpayers' money for nonappropriated purposes. Jack Crow asked if the reorganization of the field offices had any implications for the budget. Krebs said that it resulted in a 10% cut in the support of the field offices. Crow asked if it will affect the interfaces with these field offices. Krebs replied that is not yet clear. Anne Mayes asked why the appropriated amounts are sometimes higher than the requested levels of funding. Krebs responded that there is general interest in the administration and Congress to see that user facilities get used. That interest has benefitted high-energy physics. Fusion funding changed because it was cut substantially in FY 1997, and that decision has been reversed now as the result of the urging of PCAST (the President's Committee of Advisors on Science and Technology) and others. Anthony Johnson asked if there had been overtures to the Department of Defense (DOD) parallel to those to NSF, and Krebs responded that no real overtures have been made because DARPA (the Defense Advanced Research Projects Agency) has been struggling to stay even and has seen an erosion of its base support.

Richmond then called upon **Charles Shank** to review the progress of the Complex Systems Initiative. He provided an introduction and submitted the report of the workshop, Complex Systems: Science for the Twenty-First Century. The workshop was held March 5-6 in Berkeley. It was divided into five working groups addressing five research topics: unusual materials, strongly coupled systems, nonlinearity in space and time, functional design and synthesis, and the control of entropy. All five topics examine phenomena at the fundamental (atomic and molecular) scale. The chair of each group was asked to determine where this research should lead, what courses should this research take, what problems are to be solved, and how this research will benefit society and human welfare.

To organize the discussions, the workshop addressed one overarching question and four more-specific questions:

Can we exploit the new properties, phenomena, processes, and functionalities that matter exhibits at sizes between 1 nm and 100 nm?

Can we achieve an understanding of collective phenomena to create materials with novel and useful properties?

Can we design materials having predictable and yet often unusual properties, allowing us to imagine things we never imagined before?

Can we design and construct multicomponent molecular devices and machines, allowing us to make constructs to do some of the things we see done in nature?

Can we harness, control, or mimic the exquisite complexity of nature to create new materials that repair themselves, respond to their environments, and perhaps even evolve?

Some of the challenges implicit in this work are (1) whether we can develop the instruments needed to probe and exploit this world of complexity and (2) whether we can develop the computer-based theory and simulation capabilities needed to describe and predict the properties of increasingly complex phenomena. We will need to extend our capabilities to observe known phenomena, time, distance, and sensitivity. We will need new tools for detecting new phenomena and for manipulating structures.

Shank turned the floor over to **David Awshalom** to speak about collective phenomena, in which very tiny changes in the properties of matter produce very dramatic effects collectively. He focused primarily on three areas of interest: (1) strongly interacting electronic systems, (2) coherence in complex systems, and (3) quantum-phase transitions. He gave some examples to give the flavor of what happened at the workshop:

Yttrium barium copper oxide has very striking isotropy. A lot of the physics occurs in the copper oxide planes, where very minor changes in electronic doping produce very dramatic effects, such as superconductivity. What is interesting about this material is that, despite the fact that its structure has been very well identified, it behaves in a way that is difficult to understand intuitively.

Using the spin degree of freedom in materials is another evolving, interesting area. In gallium arsenide, one of the two best-studied semiconductors, long after the charge is relaxed in the semiconductor, spin behavior can occur for time and length fields that are extremely microscopic. As electron doping in this material is changed, there is a local maximum region where an optically injected packet of spin-polarized electrons precesses around a very small magnetic field for hundreds of nanoseconds. Why this persists at room temperature is not understood, but the presence of small electric fields can be seen interacting with spin-polarized packets over hundreds of microns. In contrast to charge, where very little of this can take place, the spin degree of freedom in semiconductors offers the opportunity to look at quantum coherence over long time and space scales.

Reports have appeared about growing materials to make semiconductors magnetic. In these experiments, just a few percent of magnetic ions were put into gallium arsenide, making that material ferromagnetic. This is a very important piece of technology that will have enormous impact on the $100 billion market for electronics and mass-storage devices. The phenomenon has been replicated in four or five other materials

A quantum-phase transition is the temperature between different ground states of a correlated system. These transitions offer an interesting way of looking at new materials. A major question is whether such transitions can be tuned by a parameter (such as field, pressure, or carrier density), and the answer appears to be yes. But investigating these transitions requires extreme conditions of high magnetic field or low temperature and sometimes high pressure to induce a very high level of order. In essence, the technique tries to manipulate the electronic order of solids and to use quantum mechanics to project the degrees of freedom.

Samuel Stupp then spoke on the design and synthesis of functional components, posing questions about (1) having self-organizing soft and composite matter and (2) searching for pathways to program a material to organize organic materials into functional structures. The views that emerged at the workshop were: (1) complex structures integrate many properties, (2) complexity offers a novel way to create new capabilities, (3) systems of interest include multiple-length scales and types of order, and (4) systems that mimic nature offer many opportunities. Complex functional systems hold a variety of possibilities for the development of machines that simulate the complexity of living things; the synthesis of chemically diverse nanostructures through alternative pathways to a foldable one-dimensional object; binary, ternary, and quaternary combinations of nanostructures; fresh theoretical ideas to guide the design of functional synthetic structures; macromolecular machines that can perform functions (like motion or transport); the design of catalysts to assemble three-dimensional structures (beyond the chemical-bond formation); exploring the junction of electronic/photonic material with biology (cells); and new instrumentation and tools (X-rays, neutrons, single-molecule probes, and the measurement of nanoforces). Some of these topics are best addressed by different parts of the scientific community; a major question is how to persuade those different disciplines to work together. He recommended the spontaneous formation of interdisciplinary cells drawn from universities, national laboratories, and industry.

Peter Wolynes then spoke about biology and the control of entropy in extended structures. Living things have learned to live with entropy in intelligent ways. They reproduce themselves through complex adaptive behaviors. The discipline of biology has come to understand heredity but not adaptive behavior. One way of coping with entropy is the construction of filters, as is done by proteins. The natural world has regular, cooperative systems (e.g., block copolymers), disordered cooperative systems (e.g., gels), and evolved cooperative systems (e.g., proteins and nucleic acids). Many of these materials are formed by complex processes that really are just crystallization in some very small systems that collectively produce organized structures. Thermodynamics has never been applied at the level of complexity of the cell, and there may be two or three more laws of thermodynamics still out there to be discovered. Four research paths that might be pursued are:

- the fabrication through self-assembly of highly ordered functional systems,
- the study of living systems that are highly ordered and functional (e.g., folded proteins and complex membranes),
- the study of living systems that function to produce lower-entropy entities (e.g., through photosynthesis), and
- the fabrication of structures that mimic these living systems.

Johnson asked whether there was any mention of MEMS (Micro-Electro-Mechanical Systems) or Optical-MEMS. There should be a natural transition from nanoscale structures to microscale or mesoscopic systems, with MEMS technology being one example.Wolnyes said that there was some discussion of going from the top down, starting with large items and building smaller ones. With the new advances in single-molecule science, this approach of starting from the bottom up becomes more and more possible, and he thought it would be part of this kind of program.

Franklin Orr asked if the group considered human self assembly (of interdisciplinary groups). Daniel Chemla said that is where the national laboratories come in. Awshalom said that we also need to get the best students to work on these problems. Shank noted that it also takes money to manage all these pieces. Wolynes said that language is another problem; phase transition physicists do not understand physical chemists; workshops are needed to get them together to learn the different languages and perspectives. William McCurdy asked what the next step might be, that it seems to argue for the expansion of the BES portfolio. Dehmer said that BES has small amounts that have been targeted toward these topics. A larger influx of funding would allow more interdisciplinary interaction. Marsha Lester wanted to hear more clearly the connection between the current initiative and the programs to be funded. Dehmer said that next year’s budget has not been made up yet, but it probably will go more in the direction of this workshop.

A break was declared at 10:51 a.m. Richmond called the session back into order at 11:08 a.m. to hear **William Nay** of SC to speak on security issues at the DOE laboratories. He noted that much of what the Department is responding to is in the form of presidential decision directives (PDDs), such as PDD-12, which extends the need for security awareness to all government employees, cleared or not; PDD-39, which states the nation’s counterterrorism policy to deter and preempt all terrorist attacks on U.S. territories, citizens, and facilities; PDD-61, which details the Energy Department’s counterintelligence, including making the laboratory directors directly accountable for foreign visits and authorizing the use of polygraphs in certain situations; and PDD-63, which calls for the protection of America’s critical infrastructures, such as energy, telecommunication, banking and finance, transportation, and essential government services.

He noted that the basic underpinnings of an effective security system are (1) reliable and trustworthy people and (2) training, education, security awareness, monitoring, and accountability of people and activities within the cleared system. Protecting counterintelligence interests, security interests, and sensitive information and technologies during foreign visits and assignments is a responsibility of all DOE and DOE-contractor employees. Approval of unclassified visits and assignments is the responsibility of the site manager or laboratory director with special attention paid to visits or assignments that include security areas, sensitive subjects, or foreign nationals from sensitive countries (Cuba, Iran, Iraq, Libya, North Korea, Sudan, and Syria). These measures must include indices checks, followup contact by counterintelligence officials, and compliance with the Export Control Guidelines. A 30-day advance notice for indices (affiliation checks) is required; when circumstances do not allow that latitude, the approval of the appropriate counterintelligence official must be obtained.

DOE will administer polygraphs to only individuals involved in counterintelligence activities, intelligence activities, special-access programs, personnel security, personnel assurance, and accelerated access authorization. Polygraphs will also be offered to volunteers who wish to use them for exculpation. The export control regulations do not apply to fundamental research, a classification determined largely by the intent and freedom to publish the information produced. If research is designated as “fundamental research” within any appropriate system devised to control the release of information, it will probably be treated as such by the Department of Commerce. The major technologies subject to export controls are supercomputers, hardened electronics, and high-speed electronics. The performance parameters for those computers that can be exported were recently raised. The restrictions on computer exports vary by country, and countries fall into four tiers:

- Tier 1 includes most industrialized countries; exporters are required to maintain records of exports, and re-export and retransfer restrictions apply.
- Tier 2 includes countries that pose minimal security concerns to the United States.
- Tier 3 includes countries that represent a potential proliferation or security concern.
- Tier 4 consists of terrorist-supporting states.

The cybersecurity that has emerged calls for (1) the preservation of protected data and sensitive information from unauthorized access by allowing access to only authorized personnel with a need to know, sanitizing or destroying media that have held such information, and not leaving PCs with such information unattended; (2) the standardization of banners; and (3) the regulation of e-mail (by restricting it to official business use only, prohibiting slanderous content, retaining it in archives, subpoenaing it if necessary, and monitoring it).

A break for lunch was declared at 11:34 a.m. Richmond began the afternoon session at 1:06 p.m. She said she had several positive responses to Shank's presentation during the morning session and that she wished to send a letter to Martha Krebs, urging her to support and/or expand the initiative. She also called upon the BESAC members to think of ways to promote the means and objectives of the initiative. She then introduced **Patricia Dehmer** to speak about the status and structure of BES.

Dehmer reviewed the organization chart of the Department and noted the FY 1998 appropriations of the Department's four business lines: national security (about $5.7 billion), science and technology (about $2.5 billion), energy resources (about $1.8 billion), and environmental quality (about $6.3 billion). These expenditures put DOE among the top five government research organizations for the physical sciences, environmental sciences, mathematics and computing, and engineering. In terms of expenditures for R&D facilities, DOE is the top government agency. Within SC, BES has the largest budget in the FY 2000 budget request.

The mission of BES is to (1) foster and support fundamental research to provide the basis for new, improved, environmentally conscientious energy technologies and (2) plan, construct, and operate major scientific user facilities and advance user communities for researchers at universities, national laboratories, and industrial laboratories. The office is made up of four divisions: Materials Science, Chemical Sciences, Engineering and Geosciences, and Energy Biosciences. It has a tradition of excellence in fundamental science, with 1400 peer-reviewed research projects at 200 research institutions and 18 national user facilities, including four synchrotron radiation light sources, five high-flux neutron sources, and four electron-beam microcharacterization centers.

BES's user facilities have had an unparalleled impact in visualizing the nanoworld. BES has supported innovative techniques for spectroscopy, scattering, and imaging and for 30 years has supported the talented investigators doing research on the interactions of photons, neutrons, electrons, and ions with matter. It is supporting not only programmatic research at the facilities but also R&D for the next generation of facilities. In condensed matter and materials science, DOE dominates all other agencies in terms of funding; discoveries; the development of fundamental understanding; the production of better, faster, and cheaper materials through new methods of synthesis and processing; the development of high-speed, high-resolution characterization techniques; and service to the research community. In the chemical sciences, BES operates the nation's only heavy-element program (which dates back to the early forties) and has supported research on new ideas about how to separate and synthesize chemicals. The small program supported by BES in plant and microbial sciences has had an uncharacteristically large impact, including the explication of the formation of adenosine triphosphate, which won the Nobel Prize in Chemistry in 1997. The geosciences program is the only effort in that discipline funded by DOE and has developed many of the fundamental tools of geochemistry and geophysics.

Dehmer noted that BES's budget trends show an overall, steady increase in base research, facilities operation, and capital equipment and construction [the last showing a rebound with the initiation of the SNS after the lapse that occurred with the completion of the Advanced Light Source (ALS) and the Advanced Photon Source (APS)]. She described the DOE/SC budget cycle that drives BES and all other government agencies. It starts in December with the unicall for field task proposals from laboratories and their researchers. These proposals are received in April and are used in the preparation of the corporate review budget, which through deliberation and debate is transformed into the budget request submitted to OMB in September. Feedback is received from OMB, usually on Thanksgiving Eve, and appeals of changes made by OMB are argued. The resulting budgetary data are used to prepare the president's request, which is delivered to Congress the first week of February. Congressional hearings, markups, and appeals result in a congressional appropriation in August or September, which is used by the Department to prepare an Approved Funding Program (AFP) for the fiscal year that starts October 1. Appropriate changes are made to the AFP on a monthly basis throughout the fiscal year. She showed a breakdown of the $888 million BES FY 2000 budget request by purpose: research, $395 million; facilities, $281 million; construction, $196 million; and Small Business Innovative Research (SBIR)/Small Business Technology Transfer Program (STTR) $16 million. The major change in this year's budget request was the $89 million increase (reflecting the ramping up of the SNS construction) and the $18 million decrease in the core research program (which was made up for by a similar increase in the Climate Change Technology Initiative and the Scientific Simulation Program). She highlighted the markups that had been made by the House and Senate and were being considered during the congressional break: funding for the computing initiative is gone, about 6% of the university support was allocated to earmarks, and a $19 million general reduction was imposed on BES.

Dehmer then gave an overview of the research and facilities funded by BES, noting that the BESAC Birgeneau report had reviewed the SSRL (Stanford Synchrotron Radiation Light Source), NSLS (National Synchrotron Light Source), APS, and ALS; that BESAC is soon to review the Office's four electron-beam microcharacterization centers; that the Combustion Research facility is only one of the handful of special research centers operated by BES; that the High-Flux Isotope Reactor (HFIR) was revived this past year; and the most recent construction project is the SNS, the need for which has been discussed by the neutron community for 20 years. The construction of the SNS on time and on budget is the top priority of the FY 2000 BES program; the next highest priority is the establishment of a research program in complex systems that conveys the excitement and promise of the frontiers of science. She ended by pointing out that the Office's website had been redone to make clear the connections between the research done (the research portfolio) and the sources of funding.

Sunil Sinha asked if there was a multiagency initiative on nanomaterials. Dehmer responded that Iran Thomas would address that topic in the next day's session. Stupp noted that she had mentioned cooperation among disciplines and asked how such cooperation can be brought about. Dehmer said that two means are to get them to agree what types of research to undertake and then to collocate them. The questions that will be asked will require extra resources and the top people from different backgrounds. The workshop reported that the questions require fundamental science and *more*. How should students be trained to deal with these questions? The traditional modes will still be needed but will not be sufficient. Crow asked if she had any assessment of why DOE was being micromanaged. Dehmer said that she did not. Mayes asked what the intent was for the provision of $45 million to the University of Missouri. Dehmer said that it was a Congressional directive.

Geraldine Richmond then summarized the activities of BESAC during the past several years. It was established in 1986 and

- conducts periodic reviews of BES programs and makes recommendations;
- furnishes advice on long-range plans, priorities, and strategies;
- provides guidance on the appropriate levels of funding to develop those plans, priorities, and strategies; and
- offers advice on scientific aspects of issues of concern to DOE.

It meets three to four times a year, and its members are appointed by the Secretary of Energy. Subcommittees facilitate the functioning of BESAC by investigating and making recommendations about particular matters. Recent subcommittees have considered the HFIR; light sources; novel, coherent light sources; and complex and collective systems. Each subcommittee has its own charge, panel membership, recommendations, and ongoing activities or conclusion. These subcommittees usually result from a charge letter from the director of the Office of Science to the chair of BESAC; it details the activities the subcommittee is to undertake. A subcommittee chair is then appointed and given a letter from the chair of BESAC that details what the subcommittee is to do. A subcommittee generally prepares a report that contains its findings and recommendations. The report is reviewed by the full Advisory Committee, and its formal response is sent by letter to the director of the Office of Science, after which there is sometimes a followup review by BESAC. She used the charge, membership, activities, recommendations, and subsequent responses of the Birgeneau panel (on light sources) and the Leone panel (on novel, coherent light sources) as examples of how the process works. She noted that the Leone panel has several ongoing activities: the hard X-ray region needs to be emphasized, the scientific case for coherent X-rays needs to be made; a program is needed on laser source development and applications; and an R&D program needs to be developed for the X-ray free-electron laser. She noted that BESAC had one other subcommittee in action: the review of the four electron-beam microcharacterization centers.

Joachim Stohr asked her if the Committee used formal voting or, if not, how hard decisions are made. Richmond said that the Committee both votes and reaches consensus through the work of subcommittees and through public comments and discussions. Lester asked what kind of time line Richmond envisioned for the coming year. Richmond responded that BESAC will (1) review the ALS; (2) continue the review of the electron-beam microcharacterization centers; (3) pursue the complex and collective phenomena initiative (the Committee will provide an initial response to Krebs and get further guidance); review one of the peer-and review processes in BES (probably in the spring). Lester suggested that backup material be provided prior to the meeting so that the committee members could review it. Richmond declared a break at 2:46 p.m.

She reconvened the session at 3:35 p.m., introducing **Daniel Chemla** to present a progress report and update on the ALS. In response to the Birgeneau report of BESAC, the ALS convened a users task force, which made a series of recommendations that prompted a number of actions on the part of the ALS management and its user team:

ALS was made an independent division of Lawrence Berkeley National Laboratory (LBNL).
The ALS Science Policy Board was convened.
The ALS Users Task Force was instituted.
International workshops of users were held.
A new director was selected.
International conferences were held.
A new Science Advisory Committee was instituted.
The ALS spectromicroscopy program was reviewed.

In addition, three groups that report to the director have been established: the User Services Group assists with proposal submission, establishes experiments on the floor, supports the Users Executive Committee, and helps publicize users' results; the Scientific Support Group helps users carry out experiments, assists with data interpretation, and conducts scientific outreach; and the Experimental Systems Group designs and constructs beamlines and stations, performs R&D in vacuum ultraviolet (VUV) and X-ray optics, and conducts scientific outreach.

User-group representatives now attend the weekly meetings of the management team and attend the semiannual strategic planning meetings. Users also make up a greater percentage than before of the Scientific Advisory Committee (which reviews all major proposals before submission, reviews all proposed research, and advises on resource allocation) and the program Study Panel (which allocates beamtime).

During FY 1999, $1.8 million of Laboratory-Directed Research and Development (LDRD) funding has been put into the ALS, and $4.5 million of LBNL General Plant Project funds is being used to create lab and office space. In addition, ALS user apartments are being provided nearby.

The brightness of the device gives very high energy resolution, submicron spatial resolution, and coherence. X-rays probe the optical, thermal, and structural properties of matter, which depend on the behavior of electrons. The facility's capabilities lead to excellence in research on:

many-body processes (e.g., highly correlated systems, magnetic nanostructures, and correlation in small systems);
chemistry and catalysis (e.g., wet, heterogeneous, nanoscale chemistry and biochemistry; radical dynamics; and processes at catalytic interfaces);
dynamics (e.g., at the femtosecond scale in condensed matter and the gas phase);
biosciences (e.g., large molecular complexes and structural genomics); and
tools for analysis and metrology.

Chemla reviewed some of the science being conducted at the ALS. Photoemission experiments have imaged domains on surfaces of an antiferromagnet for the first time and shown photoemission electron microscopy to be a unique tool for the study of layered antiferromagnetic materials. In determining biological structure, the ALS focuses on microcrystals and large macromolecular complexes; funding for these efforts comes from many organizations, including DOE's Office of Biological and Environmental Research (OBER), Roche Biosciences, Amgen, the University of California at Berkeley and Irvine, Lawrence Livermore National Laboratory (LLNL), LBNL, The Genetics Institute, U.S. Geological Survey, and the National Institute of General Medical Sciences. The ALS is committed to developing the techniques of macromolecular structure determination, including high-throughput crystal structure robotics (for protein purification; microcrystallization; crystal screening, mounting, and alignment; data collection; and structure determination and refinement). And ALS's high-resolution, large depth of focus extreme-ultraviolet lithography is helping to introduce advanced lithography technology into manufacturing.

The ALS has divided its roadmap into two parts: It wants to be the world leader for VUV-soft X-rays and to become world class for intermediate X-rays. All of this work is performed under high vacuum, and the development plan for any project needs to look 5 years out and to be innovative to predict the future. As a result, the gestation time for major projects is 5 to 6 years to allow time for workshops, technical design, writing and submitting proposals, undergoing proposal review, and construction.

At this point, the critical needs are:

- to build insertion devices for molecular environmental science, magnetic and polymer nanostructure research, and femtosecond spectroscopy and diffraction;
- to build end stations to study the electronic structure of correlated electron systems and to perform nanostructure characterization;
- to develop the capability to determine the time- and spin-resolved electronic structure of correlated systems, infrared spectroscopy for such systems, instrumentation and optics beamlines, and the capability to determine the structure of crystalline and noncrystalline materials;
- superbends projects for structure determination for materials chemistry, high-pressure research, micro-XAS (X-ray absorption spectroscopy), and protein crystallography; and
- infrastructure support in the form of upgraded control systems, extension of the experimental floor, a user building, detector and instrument development, and generic bend-magnet front ends.

ALS is attempting to achieve a program that is balanced between fundamental and applied science, physical and biological sciences, traditional and exploratory applications, VUV-SXR and X-ray and infrared, and spectroscopy and microscopy and diffraction, all while trying to juggle the demands imposed by unique research vs. complementary research and capacity. The ring capacity would vary drastically with the source configuration; a bend configuration would allow 30 rings, superbend 12, wiggler 3, and undulator 11. Replacing the bends with superbends, though, would produce a high flux and increase brightness to >20 keV while leaving performance at <5 keV almost unchanged, although it would reduce brightness for a couple of VUV-soft X-ray spectromicroscopes.

Two means have been set up for accessing the ALS:

- participating research teams are granted access by the Science Advisory Committee through peer review and independent investigators are granted access by the Proposal Study Panel through peer review of proposals.

The number of users has increased from 291 in FY 1997 to about 800 in FY 1999, and academic users dominate the use of the facility. The available time has been boosted by minimizing maintenance downtime, and the budget has been reorganized to decrease administrative costs and increase direct user support.

David Awshalom asked if the gestation period for new uses could be cut down. Chemla replied that it must follow a critical line to produce a good proposal. Tony Cheetham asked what the advantages were of doing X-ray crystallography on the ALS, and Chemla stated that the capacity needed is enormous and the intense beamlines are oversubscribed by a factor of 2 to 5. Sinha asked what is planned. Chemla said that the facility has only 12 magnets and that 3 will be changed to superbends; again, it is a matter of demand. Sinha asked if the demand for soft X-rays was as intense and oversubscribed, and Chemla said that the best beam lines are oversubscribed by 50%. Johnson asked if the facility gets inquiries from the pharmaceutical industry. Chemla replied that the highest demand is from that industry. Crow asked whether the pharmaceutical industry would be added to the science advisory committee given the fact of its high demand. Chemla said that it would be added. Stupp asked the cost to the pharmaceutical industry for using the facility. Chemla said that the cost varies between proprietary ($1600 per 8-hr shift) and open-literature-published research. Herbst noted that the rate of growth is spectacular. Chemla responded that in 1994, the facility was running 50% of the time. He noted also that the facility has never been completed; it has not gotten funds for the final 40% of construction.

Richmond then introduced **Iran Thomas** to review neutron science's history and future. He noted that the problem with neutrons is that they have no charge and have a spin of only 1/2; you cannot make a laser with them, and they have very low brilliance. High-flux reactors try to get 100 MW in something the size of a trash can. To overcome the heat-removal problem, pulsing was suggested in 1968. The Intense Pulsed Neutron Source was commissioned at Argonne National Laboratory (ANL) in 1981, and it is still fully operational. In 1987, R&D was started for the ALS and the APS along with the Advanced Neutron Source (ANS). The report of this Committee recommended starting R&D for a spallation source. LBNL was put in charge because it had no possibility of building it on their site. The Congress was not prepared to fund the ANS, however. The SNS project was then started to provide another high-intensity neutron source. The need for high-intensity neutrons arises from the fact that neutrons cannot be focused; rather, high peak fluxes are needed.

One idea was to bombard a target with protons from an accelerator, a concept that produced a totally new technology for making neutrons. Los Alamos decided that the Los Alamos Meson Physics Facility (LAMPF) could be adopted to make neutrons. A proton storage ring and a hall were built to make use of this facility, the basis of the Los Alamos Neutron Science Center (LANSCE). The LANSCE Reliability Improvement Project will provide more reliable operations, will extend the annual run cycle to 8 months, and will increase target power to 80 kW. A subsequent enhancement of the accelerator will increase target power to 160 kW; that enhancement will be accompanied by upgrades of the hydrogen-ion source and injector and of the proton storage ring. The latest advance at the LANSCE is HIPPO, a powder diffractometer designed for in situ study of such material properties as texture; its commissioning is expected to be complete in January 2001. With HIPPO, work that was done with an entire facility will be done with one instrument.

The High-Flux Isotope Reactor (HFIR), a beryllium-reflected, light-water-cooled and -moderated flux-trap reactor that uses highly enriched uranium (HEU) fuel was commissioned at Oak Ridge National Laboratory in 1966 with a design power of 100 MW. Every 10 years or so, the Be reflector must be replaced, so the reactor will soon be shut down for about 6 months. During that time, every instrument will be upgraded, a high-performance hydrogen cold source will be installed, and a guide hall will be added to accommodate the cold beamline. When all this is completed, the HFIR will have 14 state-of-the-art neutron-scattering instruments on the world's brightest steady-state neutron beams. BESAC's suggestions concerning the reliability of HFIR have been taken seriously. Since February 1998, it has had only one unplanned outage, which lost only two days of operating time. Its predictability has increased to 99%, and its overall availability to 63%. HFIR is also paying more attention to their biology users and has established an SNS/HFIR users group, scheduled an SNS/HFIR users meeting, and are searching for a user program scientific director.

The future of the High-Flux Beam Reactor (HFBR), a heavy-water-moderated and -cooled reactor with an undermoderated core of HEU fuel at Brookhaven National Laboratory (BNL), has not yet been determined. It is been shut down and in standby mode since Dec. 21, 1996, because of a tritium leak in the spent-fuel pool. The draft environmental impact statement (EIS, which was to have been finished in 1998) is complete but has not yet been released.

That is where neutron science is today. The future is the SNS; it will produce an order-of-magnitude greater intensity over the present capabilities.

Crow asked if there was any further statement about the status of the HFBR, and Thomas said that the Department is giving BNL $2 million per month and is reaching the point where the expenditures will outweigh the costs of restart. A decision will be needed soon. Crow said that there were rumors of the NSF's opening a second target station at the SNS and asked if DOE had any comments on this topic. Thomas said DOE has had ongoing conversations with the NSF about participation in the SNS program, but no formal agreement has been reached by the two agencies. NSF is very interested in neutron science. Sinha said that he recognized the political realities at the HFBR; BESAC was asked two years ago about the scientific need for it, but the neutron drought continues today. The SNS will not be operating for several years; it does not seem reasonable for an operable neutron facility to be kept in mothballs. Thomas responded that the path for the decision about the HFBR has been followed carefully. The EIS is an important component of that path. The Secretary has met with the scientific community and is, right now, taking all that under consideration and will make a decision. There are four alternatives: do nothing (which is not the preferred one), do a full upgrade (including the pressure vessel, but there is no funding for this), restart the reactor, and permanent shutdown. Both of the last two alternatives would require a decision and then an EIS to restart it or another process to shut it down. Financially, the project is in trouble in the outyears if we try to meet the requirements; currently, we are budgeting $23 million for operations; upgrading would cost $5 to 7 million.

Current budgets would not support that. Tony Cheetham asked who would pay shutdown costs if that option were selected. Thomas said that first it would have to be placed in safe storage until it has cooled down (about 20 years) so it can be decommissioned. Who would be responsible for it after it was put in safe storage is not known, but this process would probably cost around $5 million per year. No estimates are available at present of shutdown costs. Cheetham asked whether, if the HFBR is shut down and the HFIR is shut down, DOE has any contingency deals with the Institute Laue Langevin (ILL) or anyone else to take up the slack in providing neutrons. Thomas said the Department has had many discussions with the ILL and with ISIS and would be able to purchase time on those systems. Mayes asked what the operating costs were going to be for the LANSCE and the HFIR. Thomas said they were going to be $12.5 million for the LANSCE and about the same as current spending (or a little less) for the HFIR. Mayes asked what the timetable was for the LANSCE to come back online. Thomas said September or October. Steve Shapiro of BNL said that when the HFBR was shut down, the decision was to be made on the basis of cost, safety and science; besides the EIS, Duke Power and the Nuclear Regulatory Commission (NRC) reports have said that there would be no safety concerns. The session was adjourned at 5:28 p.m.

Wednesday, Aug. 11, 1999

Chairwoman Geraldine Richmond called the Committee to order at 8:22 a.m. She announced that the next meeting of the Committee will be Nov. 2-3, 1999, and the one after that will be Feb. 24-25, 2000, and then introduced **David Moncton** to relate progress on the SNS. He did not talk about the technical aspects of the project because the factors that threaten success are management and externalities. From the first day, he has tried to find economies so that more of the funds could be put into scientific production and so that 148,000 ft^2 could be added to the experimental facility to make it more robust.

When Congress recessed, the Senate Energy and Water appropriation stood at $187 million for the project, the House Science authorization at $118 million, and the House Energy and Water at $68 million. The project would not be able to get under way at this last level of funding. It has strong support in the House, and it is hoped that, at the end of the conference, the funding level is closer to the Senate value.

A project management assessment was conducted to develop a plan of action. It used experienced managers and independent specialists, chartered 12 teams to review different aspects of the project, and empaneled a Concept Optimization Committee to look at the fundamental concepts of the facility. The reports of these groups led to an action plan under which

- an integrated SNS organization with experienced staff has been established;
- the memoranda of agreement with the participating laboratories have been strengthened; and
- a validated technical/cost/schedule baseline has been developed to maximize the neutron-science capability, provide more lab and office space, optimize the design for operation at 2 MW, and produce adequate contingency (i.e., an estimate that is a little high in case costs come back higher than expected).

In addition, the plan called for the full qualification of the site at ORNL by the fall, the determination of the hazard category for the target (although this problem has since gone away), the development of integrated and efficient project management systems, and the tailoring of business systems to expedite and monitor the project.

The SNS director has been granted laboratory-director status, reporting directly to the Lockheed Martin Energy Research Corp. rather than through the directorship of ORNL. An SNS board of directors is planned to overcome any transitional problems during the change of contractor at ORNL. In the project organization, the project management related to construction has been restructured, and a lot of that management will go away when construction is complete. Because a lot of external influences (e.g., Congress and users) interact with the project, a number of other offices have been established in three divisions to deal with them. A staffing plan shows an increase from about 100 to about 400 employees between 1999 and 2008, with the great majority being project staff at the beginning and all being operations staff at the end. Originally, a lot of these personnel will be scattered at the partner laboratories. But as the project moves into operations, a many of them will be located in Oak Ridge. That means that the project will have to recruit a number of people from other DOE laboratories. To foster this recruitment, the SNS management has worked out variants on DOE policies so it can recruit the most highly qualified personnel. In addition, it has negotiated changes in the memoranda of agreement to define more clearly the accountability of each of the partner laboratories. These changes relate to the agreement to the technical/cost/schedule baseline; provision of human resources; development and approval of work plans; commitment to change control, configuration management, procedures, and contingency management; and accountability, reporting, and corrective actions. Under these rewritten memoranda, the SNS management may recommend performance ratings for measures in management and operating (M&O) contracts, reassign work, perform performance evaluations and make compensation recommendations at all laboratories, negotiate indirect costs, and establish fixed rates.

In the past few months, the management team has confirmed the viability of the basic accelerator concept; committed to operation at 2 MW, set a goal of 95% availability, eliminated costs of upgrade features; confirmed the viability of the mercury target (which will significantly advance the technology base); noted that the ion source has exceeded its initial design goals; confirmed that the linac design is mature and that the radiofrequency-system design and specifications are well advanced; developed a strategy for a second, low-frequency, solid target funded by the NSF; doubled the funds available for instruments and committed to best-in-class instrumentation; and finally committed to the Chestnut Ridge construction site. Johnson asked if commitment to 2 MW and narrowing the upgrade path compromises the science. Moncton said that this strategy allows the installation of better instruments, *improving* the science conducted. Upgrades just will not be made on the original schedule. He noted that it is impossible to discern today what the best upgrade options will be 20 years from now.

In other construction-related decisions, a detailed optimization of the shielding requirements and site layout significantly reduced earth-moving requirements and saved about $10 million. A strategy to accept substantial early settlement (of the building) was adopted that would not incur excessive costs or technical risks. Office, shop, and lab facilities were increased.

The site was geotechnically certified, and a record of decision was finished and signed by the Secretary, so construction may now proceed. Work on the safety documentation is now under way, and an integrated safety management system has been verified.

A review of the cost baseline showed that the budget for experiment systems has been doubled, and the cost for conventional facilities has been reduced while increasing the square footage. A table of funding scenarios showed that what happens with the FY 2000 and FY 2001 budgets will significantly affect the pace of the progress of the project. It will therefore be important to ensure that project baselines are consistent with the budget requests. The cost estimate is well documented and “owned” by the project management; a resource-loaded, integrated project schedule has been developed; contingency has been increased; and the review committee has recommended adherence to the FY 2000 budget request

At the conclusion of Moncton’s presentation, Richmond asked Iran Thomas to respond to Johnson’s question. Thomas said that, at the time that the Advisory Committee suggested the construction of a 1-MW source that would be upgradable to 4 MW, the Europeans were designing a 5-MW source. The United States wished to wait to see the results of the European R&D before designing a 4-MW source. Now the Europeans have not proceeded, and the R&D needed to produce a 2-MW source has advanced a lot more quickly than had been expected. The current strategy is to take advantage of what is known now and to go immediately to 2 MW, leaving the substantial upgrades (to 4- and 5-MW operating powers) to technologies to be developed later.

Moncton noted that the facility will not operate at 2 MW immediately; but within 2 years of the first proton’s being produced, it will achieve the 2-MW power level. However, the cost implications of the length of time over which the power is increased to 2 MW are significant.

Stohr asked if he understood correctly that the senior management of the project is located at Oak Ridge but that it will do performance evaluations at other laboratories. Moncton said that it was correct that the lines of authority cross laboratory boundaries. Usually, however, the performance appraisals will be performed by a person’s immediate supervisors. So, at some point, the line of authority crosses from someone who is an Oak Ridge employee to one who is, say, a Los Alamos employee. Once an employee is in another lab, the performance evaluations are done by that lab’s supervisors. It is only one appraisal that goes across the boundary.

Goodman asked if there were any problems in the contractor transition at ORNL and if all the potential contractors were discussing the plans for the SNS with the project management. Moncton said that he has had more discussions with one potential contractor than the other, but that he is available for further discussions. One of the problems that could arise might be very significant changes in management philosophy and approach. Whether that happens depends on what team is selected and its philosophy. The proposal revision process has only just begun.

Crow moved to commend Moncton and his team for the effort, commitment, and progress shown. Herbst seconded, and the motion passed unanimously.

Richmond moved on to nanoscale science. Thomas said that the National Science and Technology Council had a council on nanoscale science and DOE has been represented on that council. BES decided that it needed something to indicate what the office should be doing in nanoscale science and technology. Also, the president's science advisor sent a letter to the agencies telling them that they should be paying attention to, and one of those topics was nanoscience. Therefore, BES had a report compiled as a prelude to a nanosciences initiative, a subset of the office's physical sciences initiative. He introduced **Douglas Lowndes** from ORNL to talk about that report.

He noted that an interagency working group on nanoscience has authored *Nanotechnology for the Twenty-First Century: Toward a New Industrial Revolution*. That interagency report has not yet been published, but its executive summary has been circulated. It suggests that NSF and DOE should be provided the largest budgets for nanoscience research; that federal spending on nanotechnology should be doubled; that research on nanoscale science, engineering, and technology (NSET) will be highly interdisciplinary and collaborative; that a substantial long-term impact will result (comparable to that of computers); and that research leading to a fundamental understanding and discovery of phenomena, processes, and tools for nanotechnology should be emphasized. It identifies several modes of support needed:

- capital and infrastructure development at the national laboratories,
- funding of universities for collaborations with DOE laboratories,
- funding of national laboratories to work with other government agencies and (later) with industry, and
- formation of several nanoscience/engineering/technology user facilities at national laboratories.

Concurrently, BES requested its Nanoscience/Nanotechnology Group to write a report about the anticipated national, interagency research initiative being deliberated by the interagency working group. The DOE/BES report is entitled *Nanoscale Science, Engineering, and Technology: Research Directions.* It describes important future research directions in NSET. It illustrates the wide range of research opportunities and challenges that can be undertaken, the questions to be answered, and the kinds of research activities to be undertaken. The objectives of the DOE/BES report are to ensure the effective use of DOE resources and BES leadership in NSET. It covers such topics as:

- emergence of properties at multiple length and time scales,
- manipulation and coupling of properties at the nanoscale,
- controlled synthesis and processing at the nanoscale,
- nanoscale precursors and assembly for macrostructures and devices,
- understanding and mimicking biological functions,
- hybrid systems: integrating functionality,
- nanoscale instrumentation, and
- infrastructure and facilities for nanoscale science and technology.

It also contains an appendix describing the formation of nanomaterial research centers.

The report suggests that, during the next decade, science will have a unique opportunity to understand and control materials properties from the nanoscale upward. New synthesis methods will permit atomic and electronic structure to be controlled near the atomic scale, in one, two or three dimensions. The development of instrumental probes will progress to measure both structure and properties on a wide range of length and time scales. At the same time, the explosive growth of computational power will permit the theoretical study of structure-property relationships on all length scales.

The report identifies three key science and engineering challenges: the need to understand

- how new properties of materials will emerge on the nanoscale,
- how to deliberately tailor materials on the nanoscale to achieve new or enhanced functionalities, and
- how to couple properties across multiple length and time scales (e.g., assembling nanoscale "building blocks" for macroscale materials).

Science has a reasonably good idea of how properties emerge at the nanoscale. One mechanism is the effect of size constraints, which produce qualitatively new behavior. If the nanostructure size is less than the characteristic scattering length (the mean free path), new modes of electrical current or energy (heat) transport are possible. If the nanostructure size is less than the coherence length or quasiparticle size, then collective phenomena, phase transitions, and thermodynamic properties are strongly modified. Examples are ferromagnetism, ferroelectricity, superconductivity, large "molecular magnets," and ultrathin films (quasi-2D magnets). The message here is that there exists an opportunity to tailor properties of materials that are 0.1 nm to tens of nanometers.

The characteristic time scale shifts for nanoscale phenomena partly because of the length-scale change; characteristic frequencies increase with shorter transit times (at fixed electron, phonon, or photon velocity). Genuine changes of regime also occur (such as the increased importance of surface phonons vs. volume phonons and ballistic electron transport). An increased rate of kinetic processes is caused by (1) an increased fluctuation rate with decreasing system size and (2) an increased surface-to-volume ratio. As a result, there should be increased sensitivity and reduced response time for sensor elements in biological and chemical systems. We need to learn how to exploit large surface-to-volume ratios, but it will require instrumentation with improved time resolution and ultrafast probes.

In addition, new properties are expected to emerge because quantum-mechanical tunnelling will be significant over such short distances, quantum confinement will shift electronic energy levels, and surface-to-volume ratios will become very large.

The emergence of new phenomena will create a strong need for theory, modeling, and simulation. Structure-property linkages are not well understood at the nanoscale; we would like to be able to link electronic, optical, magnetic, and mechanical properties with size, shape, topology, and/or composition. [An exception is that considerable progress has already been made for the electronic properties of the simplest systems (e.g., semiconductor thin films and carbon nanotubes).] However, for composite materials and hybrid structures, the basic outlines of theory are lacking. Computer simulations will play a major role in materials design and assembly. And opportunities for theory and modeling will occur at several length scales, with the greatest opportunity at the transition where nanoscale phenomena just emerge.

Some key scientific questions related to the controlled synthesis and processing at the nanoscale are:

- Can single-wall carbon (or other) nanotubes of specific length and definite helicity be purified (or grown) as isolated molecules?
- What are the surface reconstructions in nanocrystals and nanorods?
- Can heterojunctions be prepared reproducibly from 1–D nanostructures?
- Can parallel self-assembly techniques control the arrangement of nanoscale components according to a complex, designed sequence?

The importance of nanotechnology for energy science lies in the facts that:

- Transport phenomena (such as electron transfer and exciton diffusion) occur on the nanometer scale.
- Nanometer-size "building blocks" are being discovered and developed.
- Isolated nanoscale components exhibit near-ideal mechanical and electrical properties.
- Inexpensive methods need to be developed for nanometer-scale patterning, processing, and assembly in order to produce improved next-generation photovoltaic cells and batteries.
- Methods are needed to (self-) assemble these components into complex, hybrid materials so that energy technologies (such as catalysis, photovoltaics, and batteries) can be transformed.

The panel's principal conclusion is that there is a strong synergism between the NSET initiative and DOE's missions and research needs. For example, nanoscale synthesis and assembly are expected to yield improved solar energy conversion; more-energy-efficient lighting; stronger, lighter materials; improved transportation efficiency; greatly improved chemical and biological sensing; low-energy chemical pathways to break down toxins; better sensors and controls for increased manufacturing efficiency. DOE's Office of Science is already strongly focused on enabling scientific discovery, supporting research to develop fundamental scientific understanding, and converting both into useful technological solutions. And the panel found that DOE is well prepared to provide a major contribution to the NSET interagency initiative because:

- It has an outstanding array of large-scale, multiuser neutron and synchrotron X-ray sources; analysis and characterization facilities; and nanointegration facilities.
- Stewardship is a specific mission of DOE's Office of Science.
- Its synchrotron X-ray and neutron sources produce a wavelength and energy range that is ideally suited to study nanoscale structures, and the high flux of sources permits a very wide range of studies.
- Its electron-microscopy and electron-diffraction capabilities are indispensable for near-atomic-scale visualization of nanomaterials, and its facilities have additional capabilities for nanoscale property measurements.

However, there are barriers to using the major national facilities for nanoscale research:

- Reliability is essential for productive research by external onsite users.

- A fundamental challenge for nanotechnology is implementing a hierarchical linkage across multiple length and complexity scales; it is both a scientific and a technological challenge to bring together characterization facilities, synthesis and processing tools, and interdisciplinary technical expertise.
- Significant investments in ancillary equipment (nanomaterials synthesis, processing, and characterization facilities) will be needed, and they will need to be closely associated with major X-ray, neutron, and nanointegration facilities.

The most effective use of such facilities would require a dedicated team of onsite scientists actively pursuing nanoscale research. The national laboratories would provide an ideal setting because major characterization facilities are already in place there. The research should be focused by establishing several nanomaterials research centers that would use DOE's national facilities for nanomaterials synthesis and characterization, nanostructure fabrication, and nanotechnology integration. Each center would have a primary focus, such as materials derived from or inspired by nature; hard and crystalline materials (including the structure of macromolecules); magnetic and soft materials (including polymers and ordered structures in fluids); or nanotechnology integration. Such centers would address four needs: facilities, research organization, support for external users in terms of infrastructure and collaboration, and education of a new generation of scientists in an interdisciplinary manner.

In summary, the DOE/BES report notes that:

- There are strong overlaps between nanoscience research and other BES priorities.
- Nanoscience research is highly interdisciplinary and collaborative, and the key advances will occur at interfaces between disciplines.
- The nanotechnology initiative may be another step in the evolution of the national laboratories toward becoming a unified system of national resources.

Collin Broholm noted that there was no one from industry on the committee that wrote the report. Lowndes replied that the report was for the BES and was intended to scope out how it should proceed; the interagency group has many representatives from industry and they provide major input. Awshalom asked what plans they had for increasing human resources. Lowndes responded that that was outside the committee's charge; it would be the responsibility of BES and other institutions and agencies to determine staffing needs; the committee sees the national laboratories reorganizing to form interdisciplinary groups. Herbst asked if there were any thoughts about hydrogen storage. Lowndes said that that is one of the important research objectives. Zhi-Xun Shen asked if he had thought about how to couple the activities he emphasized here, commenting that no new phenomena had been seen at the nanoscale during the past decade and that there did not seem to be a strong technological attraction here. Lowndes replied that the focus is clearly on nanotechnology but, in the first 10 years, industry cannot be expected to bear the costs to discover phenomena like those described. Regarding new nanoscale phenomena, Lowndes thought that this situation was changing very rapidly.

Johnson asked if there could be a fellowship program in nanoscale science and technology, particularly for minority women. Lowndes said the group would strongly favor that, but the decision would be up to the program office.

Paul Alivasatos presented a report on the DOE Workshop on High-Pressure Science, jointly sponsored by the Council on Earth Sciences and the Council on Material Sciences. The workshop was held June 12-13 and was the first to be held on the subject since 1982. The key conclusion was that the field is evolving very rapidly at the moment because static, equilibrium properties of solids can be studied and described extraordinarily well theoretically. There appear to be pathways to attain ultrahigh pressures and temperatures in the terapascal regime by a variety of techniques. This community calls this the regime of warm dense matter and says that new physics can occur here at the intersection of condensed matter and dense plasmas. Some of the questions they have talked about are:

What are the properties of metallic hydrogen?
Can any phase transitions occur in plasma?
What are the physics and chemistry of planetary cores?

There are important connections to the materials area, connections that occur at several levels. New phenomena might be discovered (e.g., new states of electronic and magnetic order might occur at ultralow temperatures and multimegabar pressures). A lot of people at the workshop talked about performing combinatorial studies of phase diagrams inside diamond cells. We can use pressure to tune the optical or magnetic properties of materials to optimal low-density compositions. The alteration of chemical bonding yields new families of solids (mixtures that do not react at room pressure form compounds at high pressure; for example, potassium and argon react to form solids). High-pressure studies may also lead to an improved understanding of metastability; nanostructures are defect-free model systems for solid-state kinetics, and high-pressure science will therefore have a strong coupling with these nanostructure models.

Significant interest was expressed in theory. The whole field is resting on the foundation that density functional theory and quantum chemistry both can provide pretty accurate calculations of what are static equilibrium structures and they make it possible to predict those structures. There is also the hope that the control of matter on multiple time and length scales will feed back into this and allow theory to progress.

New technologies are emerging from these studies, such as the development of

techniques to probe time-dependent phenomena under high pressure,
designer anvils for multimegabar pressures, and
combined static and dynamic compression techniques.

All of this work will depend heavily on third- and fourth-generation synchrotrons. Currently, there is not enough capacity on these machines for doing the type of high-pressure work that needs to be done, and we look forward to being able to do dynamics with X-ray diffraction experiments.

Stupp asked why he emphasized experiments at the nanoscale and what the advantage was to the use of the combinatorial approach to phase diagrams. Alivasatos said that very small materials tend to be defect-free materials and that the ability to map composition in parallel makes the task of developing phase diagrams go a lot faster. Mayes commented that he should keep in mind the great opportunities at the SNS. Alivasatos said that he meant to mention that.

A break was declared at 10:29 a.m. Richmond called the committee back to order at 10:47 am and introduced **Tony Cheetham** to report on the workshop on partially ordered chemical systems, which was sponsored by the Chemical Sciences Division of BES and held May 10-14, 1998. He noted that the subject has an enormous scope because of the different length scales (from 1 Å to 10 µm) and dimensionalities (zero to three dimensions). DOE is interested in these materials because they are used in hydrogen storage, superconductivity, magnetics, batteries, fuel cells, catalysis, sensors ceramics, electro-optics, structural materials, and separations. The workshop covered materials with different types of disorder, tools used for characterization by scattering and spectroscopy, and the roles of theory and simulation. Considerable attention was paid to zeolites: their disorders, framework, charge-coupling state, and absorbed molecules. A multifaceted approach that includes simulation, spectroscopy, calorimetry, and diffraction is needed to investigate these materials, and sometimes these techniques will give opposing and contradictory results. The workshop also addressed the dynamics of semi-ordered systems, including microscopic diffusion at or on surfaces, bulk diffusion and transport, cation migration and exchange, and chemical (molecular) dynamics. For these studies, electron microscopy can provide spatial resolution of the structure (e.g., single-crystal data on a precipitate 10 nm on edge), chemical composition, and other properties, allowing models to be constructed. At the other end of the size spectrum, studies of activated carbon have found that the material's disorder can be fine tuned to differentiate between nitrogen and oxygen. Examination of biomaterials reveals long-range order with terrific disorder at the local level. For example, biology has evolved unique mechanisms for the catalysis and organization of silica polymerization. The tools needed to study these semi-ordered systems include current national user facilities (e.g., synchrotrons, neutron sources, the National High Magnetic Field Laboratory, nuclear magnetic resonance imaging, and the Environmental Molecular Sciences Laboratory) and the development and adaptation of new tools (e.g., soft X-rays; reflectometers; low-frequency, high-resolution, inelastic-neutron-scattering stations; and nuclear magnetic resonance). The workshop discussed future directions of theory and modeling, including integrated structure refinements, structure-image relationships, and novel mesoscale approaches. The main goal here is to show a clear integration between simulations and experiments. The key recommendations of the workshop were:

- the major user facilities should be exploited in characterizing these materials,
- combined approaches [e.g., diffraction plus nuclear magnetic resonance (NMR)] should be employed in characterization,
- real-space and reciprocal-space strategies should be combined in characterization efforts,
- first principles rather than force fields should be emphasized in preparing simulations,
- simulations should be better integrated with experiment, and
- theory should guide synthesis.

Richmond introduced **John Stringer** to review electron-beam centers. Electron beams make a unique contribution to material analysis that supplements (and sometimes duplicates) information from photon and neutron analyses. Electrons make a good contribution to the analysis of impurities. The panel is looking at the four electron-beam microcharacterization centers supported by BES to assess the science and technology impact of the centers. Questions to be considered are: What is the user demand and how will it change? What special needs do the centers serve? What are the opportunities for improving the techniques? What is the vision of each center?

The centers are justified by the quality of the science, enabling scientific investigation that would not otherwise be done. These topics will be discussed in a meeting, and then the panel will visit the four sites. He reviewed the membership of the panel and the qualifications of those members. Its initial meeting is on Friday, August 13. The directors of the centers have assembled a document, *Electron-Beam Characterization Centers: A National Resource*, specifying and detailing work that is done by the centers.

Dehmer said it would be good if the panel would complete its work by February. Stohr asked where these centers are. Stringer replied: ANL, ORNL, University of Illinois, and University of California at Berkeley. Stohr asked if this was the first review. Stringer replied that there had been two others, one of which left no report. Mayes asked if the panel had any expertise on biology, and Stringer said biology is supported by NIH and the charge excluded us from looking at biological materials.

Richmond asked for public comment, but there was none. She will send letters to Krebs supporting the Complex Phenomena Initiative and commending the progress on the SNS. She adjourned the meeting at 11:49 am.