Minutes of the
Basic Energy Sciences Advisory Committee Meeting
February 25-26, 2002
Gaithersburg Marriott Washingtonian Center, Gaithersburg, Maryland

BESAC members present:

Collin L. Broholm
Patricia M. Dove
Laura H. Greene
Walter Kohn
Gabrielle Long
C. William McCurdy, Jr.
Daniel Morse
John Richards
Zhi-Xun Shen
Rudolf Tromp
Jack E. Crow
D. Wayne Goodman
Anthony M. Johnson
Marsha I. Lester
Anne M. Mayes
C. Bradley Moore
Ward Plummer
Geraldine L. Richmond, Chair
Samuel I. Stupp

BESAC members absent:

Philip Bucksbaum
Mostafa A. El-Sayed, Vice Chair
Cherry Murray
Sunil Sinha
Kathleen C. Taylor
James A. Dumesic
George Flynn
Richard E. Smalley
Joachim Stohr

Also participating:

Mark Alper, Deputy Head, Materials Sciences Division, Lawrence Berkeley National Laboratory
Eugene Bierly, Director for Education and Research, American Geophysical Union
James Decker, Acting Director, Office of Science, DOE (Thursday only)
Patricia Dehmer, Director, Office of Basic Energy Sciences, DOE
Fred Gilman, Head, Department of Physics, Carnegie-Mellon University
Keith Hodgson, Director, Stanford Synchrotron Radiation Laboratory, Stanford University
Linda Horton, Associate Division Director, Metals and Ceramics Division, Oak Ridge National Laboratory
William Kirchhoff, Office of Basic Energy Sciences, DOE
Carl Lineberger, Department of Chemistry and Biochemistry, University of Colorado
Paul W. Lisowski, Director, LANSCE Division, Los Alamos National Laboratory
Thom Mason, Director, Spallation Neutron Source, Oak Ridge National Laboratory
James Roberto, Associate Director, Oak Ridge National Laboratory (Tuesday only)
Ned Sauthoff, Head, Off-Site Research Department, Princeton Plasma Physics Laboratory
Marvin Singer, Director, Office of Advanced Research, Office of Fossil Energy, DOE
Walter Stevens, Office of Basic Energy Sciences, DOE
John Stringer, Executive Technical Fellow, Electric Power Research Institute
Iran Thomas, Director, Division of Materials Science, Office of Basic Energy Sciences, DOE

Monday, February 25, 2002

Chairwoman Geraldine Richmond called the meeting to order at 8:35 a.m. She had each member introduce himself or herself. She then welcomed **James Decker**, Acting Director of the Office of Science (SC), who presented an update on the operations of SC. He noted that Ray Orbach's confirmation hearings as Director of the Office of Science were to be the next day. The Department's budget request for FY 03 is up $582 million, with the requests for the National Nuclear Security Administration up $433 million, Environment up $169 million, Science up $5 million, and Energy down $78 million.

Not factoring in the Spallation Neutron Source (SNS) and the one-time FY 02 projects, Science is requesting a 5% increase. Significant differences in this budget include:

- Science thrust areas:
  - Nanoscale Science, Engineering, and Technology (at $133 million, an increase of $48 million)
  - Genomes to Life (at $45 million, an increase of $20 million)
  - Climate Change Research Initiative (at $3 million, an increase of $3 million)
  - Scientific Discovery Through Advanced Computing (SciDAC; at $62 million, an increase of $5 million)
- More operating time and new instrumentation at user facilities (at $1246 million, an increase of $40 million)
- Improved infrastructure at ten of the Department's laboratories (at $43 million, an increase of $6 million)

He provided budget totals for all the offices within SC for fiscal years 2001, 2002, and 2003 and noted that all congressional initiatives in FY 03 are in the Office of Biological and Environmental Research (OBER).

In the Office of Basic Energy Science (BES), the requested funding for research is $488 million, an increase of $37 million, $17.5 million of which is for improved instrumentation for the SNS. That for facilities is $279 million, an increase of $10 million. That for construction, engineering, and design includes full funding for the construction of the SNS at $211 million; the nanoscale science research centers (NSRCs) at Oak Ridge National Laboratory (ORNL), Lawrence Berkeley National Laboratory (LBNL), and Sandia National Laboratories/Los Alamos National Laboratory (SNL/LANL) at $11 million; and the NSRC at ORNL at $24 million. It also includes project engineering and design of the Linac Coherent Light Source (LCLS) at the Stanford Linear Accelerator Center (SLAC) at $6 million. The LCLS will be a fourth-generation light source [an X-ray free electron laser (XFEL)] that will serve as a research and development center in the hard X-ray regime and as a facility for experimental studies of structure and function of chemical, physical, and biological systems.

In the Office of Advanced Scientific Computing Research (ASCR), not much is new. The Mathematical, Information, and Computational Sciences (MICS) Program will continue to support the operation of supercomputer and network facilities; scientific computing research investments in applied mathematics, computer science, and advanced computing software tools; high-performance networking, middleware and collaboratory research investments; and laboratory technology research. Within this program, SciDAC is building community simulation models through collaborations among application scientists, mathematicians, and computer scientists to produce research tools for

plasma physics, climate prediction, combustion, etc.

In OBER, the major emphasis is on Genomes to Life, which will enable revolutionary advances in energy supply, greenhouse gas mitigation, and environmental cleanup; its requested funding is $37 million, an increase of $15 million. The Human Genome Program will complete the sequence of chromosomes 5, 16, and 19. The Climate Change Research Initiative will improve climate models and the understanding of the global carbon cycle and will enhance carbon sequestration; its requested funding reflects a $6 million increase. The Environmental Management Science Program is being transferred from the Office of Environmental Management (EM) to SC. Boron Neutron Capture Therapy is being wrapped up, and the research is moving to the National Cancer Institute (NCI).

In Fusion Energy Sciences, the overall budget request is $10 million more than last year, but there is a roll-off because of completion of the tokamak at Princeton. The major devices will be brought up to full operation, and design will be started for the national Compact Stellarator Experiment, which combines tokamaks and stellarators.

In High-Energy Physics, the budget remains very tight with an increase of $10 million. The Alternating Gradient Synchrotron (AGS) at Brookhaven national Laboratory (BNL) is being terminated. Emphasis is on enhancing the capabilities of the Tevatron at Fermilab and increasing the operating time and capability for the B-Factory at SLAC. These efforts include upgrades of the accelerators and detectors at those facilities and the construction of the Neutrinos at the Main Injector (NuMI) facility at Fermilab, increasing the construction budget by $9 million.

In Nuclear Physics, the budget request would increase overall funding by $23 million overall, allowing the Heavy-Ion Collider at BNL and the Continuous Electron Beam Accelerator Facility (CEBAF) at the Thomas Jefferson National Accelerator Facility to operate at full capacity.

The FY 03 budget request would increase funding for critical infrastructure improvements and support the removal of excess facilities.

The President's Management Agenda emphasizes the management of scientific programs very much. In a speech to the American Association for the Advancement of Science (AAAS) on Feb. 15, 2002, Jack Marburger said, "The President's budget makes much of management, and proposes many measures that are not particularly designed to save money so much as to optimize its impact . . . the growth in opportunity requires better decision making. I support these science management initiatives [as they apply to federal investments in science]." The Administration is focusing on improving the performance of all R&D programs in the preparation of the FY 04 budget; investment decisions will be based on transparent investment criteria. The Administration is using the DOE Energy programs as a pilot to develop investment criteria for applied R&D programs. The Administration also recognizes that the goals and methods of basic research are different from those for applied R&D and is working to define an appropriate set of criteria. OMB [Office of Management and Budget] rated all government agencies in effectiveness, and two DOE offices were singled out as being well managed: the National Nuclear Security Administration and the Office of Science.

Decker said that he was looking forward to receiving the BESAC report on performance measurement. It will inform the discussion at the Workshop on Investment Criteria for Basic Research, which will be held Feb. 27, 2002, and be sponsored by the Committee on Science, Engineering and Public Policy (COSEPUP) of the National Academy of Sciences. It will also inform future management reviews.

Kohn referred to a prior comment and asked how Genome to Life will lead to advances in energy

supply. Decker replied that there are microbes that produce hydrogen, a fuel, and biofuels of several types. Consideration of such microbes as fuel sources is at a very early research level. Kohn asked where this is being done. Decker said, at the National Renewable Energy Laboratory (NREL) and several other laboratories and universities.

Kohn pointed out that the National Ignition Facility's (NIF) funding was not mentioned in the presentation. Decker said that SC does not have anything to do with the funding of NIF, but it is an important experiment for fusion energy. It is on the defense side of the Department.

Richmond introduced **Patricia Dehmer** to present an update on the Office of Basic Energy Sciences. Dehmer identified a variety of activities that the Office and BESAC were engaged in. The BES portion of the President's Request to Congress for FY 03 was developed. The Committee of Visitors for BES Chemistry Programs looked at chemistry research at the universities and laboratories, about 30% of the research funding. The committee assessing performance measurement in SC will feed into a workshop on investment criteria later this week. The Biomolecular Materials Workshop, the first in a series of bio-nano workshops, was held.

A Workshop on Basic Research Needs for Counterterrorism is in the planning stage. A Workshop on Future Directions in Catalysis will be held in mid May. A Workshop on the Computational Nanosciences will be cosponsored with the Advanced Scientific Computing Advisory Committee (ASCAC). And a workshop will be conducted on Basic Research Needs for Energy Security.

She reviewed the role of advisory committees in SC and how they aid program assessment and long-range planning. She noted the publications that have come out of BESAC's activities and commented on their individual significances and effects, underscoring the fact that BESAC has had a major role in the development of the BES program.

The FY 03 requested budget funds are distributed among research at universities ($175.9 million), research at national laboratories ($231.9 million), user facilities ($244.6 million), capital equipment ($76.2 million), general plant project (GPP; $12.6 million), construction ($251.6 million), and Small Business Innovative Research/Small Business Technology Transfer (SBIR/STTR; $17.7 million).

She quoted from John Marburger's speech, Science Based Science Policy, presented at the AAAS on February 15, 2002: "The quantum technologies of the chemistry and physics of atoms, molecules, and materials developed rapidly through several generations during the Cold War. By 1991, when the Soviet Union finally dissolved, scientists were beginning to wield instruments that permitted the visualization of relatively large-scale functional structures in terms of their constituent atoms. The importance of this development cannot be over-stated. The atom-by-atom understanding of functional matter requires not only exquisite instrumentation, but also the capacity to capture, store, and manipulate vast amounts of data. The result is an unprecedented ability to design and construct new materials with properties that are not found in nature.

> "The revolution I am describing is one in which the notion that everything is made of atoms finally becomes operational.
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> "This revolution is caused by two developments: One is the set of instruments such as electron microscopy, synchrotron x-ray sources, lasers, scanning microscopy, and nuclear magnetic resonance devices; the other is the availability of powerful computing and information technology. Together these have brought science finally within reach of a new frontier, the frontier of complexity.

"The picture of science I have portrayed -- and I am aware that it is only part of science, but an important part -- has immediate implications and challenges for science policy.

"First, there is the need to fund the enabling machinery for exploring the frontier of complexity. Some of this machinery is expensive, such as the great x-ray sources operated by the Department of Energy, or the Spallation Neutron Source. Even the computing power required at the frontier is expensive and not yet widely available to investigators.

"Second is the desirability of funding research in the fields that benefit from the atomic level visualization and control of functional matter. They fall into the two categories of organic and inorganic. We call them biotechnology and nanotechnology. I like to think of biotechnology as organic nanotechnology.

"Third, there is the very serious problem of the inadequacy of resources to exploit all the new opportunities that now lie before us along the vast frontier of complexity. The need for choice, and for wise allocation of resources to seize the most advantage for society from our leadership in these fields, is a strong motivation for better planning and management of the nation's science enterprise."

Dehmer commented that this speech outlined three tenets for good planning: make sound investment choices, make sure that extant facilities are maintained and instrumented well, and explore promising fields like biotechnology. The increases in the FY 03 budget request reflect these tenets.

There are increases for science at the nanoscale in condensed-matter physics, materials synthesis and processing, and catalysis and further increases for project engineering and design (PED) funding of nanoscale science research centers at ORNL ($1.0 million), LBNL ($6.8 million), and SNL/LANL ($3.2 million). Construction funding is provided for the Center for Nanophase Materials Sciences (CNMS) at ORNL ($24 million). The facility will be collocated with the SNS. Following construction, future research budgets will be of a magnitude to fund research staff and support staff for users. She pointed out that DOE Order 413.3 defines how construction is to be managed. The process has five major processes, each followed by a critical decision (CD). The first phase, preconceptual planning, is followed by CD-0, the approval of mission need. Three of the NSRCs have a signed CD-0, and their conceptual designs have begun.

There are increases in the budget request for other BES activities with relevance to beyond-nano and to core-mission areas, such as materials chemistry, photochemistry, separations science, and heavy-element chemistry. There are increases (averaging 5.8%) for facility operations, upgrades, and construction. The High-Flux Isotope Reactor (HFIR) and the SNS are the only user facilities experiencing an overall decrease in the FY 03 budget request; HFIR's upgrade is complete, and the SNS's construction peak is past.

The budget includes funds to increase operations at synchrotron-radiation light sources, neutron-scattering facilities, and the combustion research facility; the completion of the SPEAR-3 [Stanford Positron Electron Asymmetric Ring] upgrade; full funding for the SNS; and $6 million in PED funding for the LCLS, which BESAC has looked at quite intensively during the past years. There are significant increases for major instrumentation, specifically to support instrument upgrades, instrument replacements, and new instrumentation at the x-ray and neutron scattering facilities. $5 million will be provided for instruments at the SNS. These funds will be competed among both academic and laboratory institutions, and the resulting instruments and beamlines will be made available to the entire U.S. scientific research community. Also, there is an increase in ASCR's

budget for computational nanosciences that affect BES's activities in nanoscience.

She reviewed the DOE/SC budget cycle and pointed out that if one wants to affect the FY 04 budget, one has to do it soon.

The Office was asked to write a short piece for *Science Next Wave* (online), and Iran Thomas wrote up what the basic research needs are for each energy-source center. In anticipation of a workshop on needed energy research, the Office would like to have the Committee's help in categorizing the different advances that are being pursued and the research that will be needed.

She closed with a look at the recent changes in personnel at BES.

Stupp asked what the objective of the workshop would be. Dehmer replied: to understand the breadth of new energy research needs. That is what BES does for a living. It needs to identify areas in which in-depth workshops might be held.

Crow stated that power-engineering manpower training has been abandoned by universities and asked if any workforce issues would be addressed in this workshop. Dehmer said that workforce issues will be an important point. Every agency that funds research has an obligation to address the problems of human resources.

Moore asked for clarification that the counterterrorism workshop is different. Dehmer affirmed that it is separate.

Kohn asked if the documents that underlie the research-needs workshop are available. Dehmer said that she did not know; the organizers have had to rethink them in terms of the President's Management Agenda. Kohn asked what energy security is. Thomas responded that the United States spends a large amount of money protecting our energy supplies. Kohn asked if he meant in a military sense. Dehmer said, no; this is one block of national security. Kohn noted that Lawrence Livermore National Laboratory (LLNL) has had its budget for civilian power dwindle and asked if funding would be available down the line for that area and at what amount. Dehmer said that she would not want to give such a number.

Mayes asked if the cited increases are enough to support outside users of facilities. Dehmer observed that the major impact on the use of facilities by outside users is the number of resident scientists. BES is trying to move staff into those positions to make a good program available to outside users.

Richmond declared a break at 9:59 a.m. and called the meeting back into session at 10:17 a.m. to hear **Carl Lineberger** present a preliminary report on the activities of the Committee of Visitors (COV).

The charge to the COV is to establish a committee of visitors through which BESAC can provide an assessment on a regular basis of matters pertaining to program decisions. The COV should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs and to comment on how the award process has affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements. The COV is to comment on future directions and on how the process for these reviews might be improved.

The National Science Foundation has used COVs, but their model has to be modified to apply to a mission agency.

The tasks were divided among four groups. Group 1 looked at (1) Atomic, Molecular, and Optical (AMO) Physics and (2) Chemical Physics. Group 2 looked at (1) Photochemical and Radiation Sciences and (2) Electrochemistry. Group 3 looked at (1) Separations and Analysis and (2)

Heavy Element Chemistry. Group 4 looked at (1) Catalysis and Chemical Transformations and (2) Chemical Engineering.

The COV is made up of 20 experienced, well respected individuals. About 25 % receive no DOE support. A balance is attempted among research area, university investigators and national laboratory investigators, and those with (or without) prior DOE/NSF program-management experience. The COV process includes a general overview BES presentation to the full COV, separation into the expert groups, meeting with appropriate program managers, evaluating jackets by requested criteria, and the drafting of a report from each group. Those reports are read by the members of another group, and they review the same materials to provide a crosscutting reality check, looking at research quality standards and procedural standards. The findings of the two groups that review each program are merged to produce a final group report. The COV then meets as a whole to identify common issues.

Each group received documents covering the BES mission relevance for all projects; the FY 1998, 1999, and 2000 budgets; approximately 12 university-program jackets; a listing of all active projects; several easy-fund and easy-decline cases (most jackets were at the decision margin); all the national-laboratory jackets; new initiatives; proposals, site visits, and recommendations; continuing projects; and site-visit reports, reviews, staff recommendations, and laboratory responses.

As part of its general observations, the COV strongly commends Pat Dehmer for taking the lead in establishing this oversight process to improve and open programs. Staff support for the COV was excellent. The research portfolios are of very high quality. The research programs are, in general, well managed and carrying out important, relevant science for DOE.

The COV made general recommendations in five classes: standardized program documentation, program-evaluation mechanisms, program quality, BES staffing and program support, and the COV process itself.

Under standardized documentation, the COV recommended that BES develop common forms for referee reports, solicitations, and all other repetitive activities. It should design the report form to force a recommendation. It should develop a time/document-line page for the front of every project jacket to enable the ready determination of what actions, responses, and materials are present. This cover page should include all important events in the project and make apparent when something did or did not take place. The university-program documentation follows long-established procedures, and project documentation is generally appropriate and complete. In the national-laboratory-program documentation, new initiatives are generally well-documented, but continuing-program documentation is less complete. The laboratory responses to site visits and to DOE recommendations are often verbal rather than written, and the emphasis is on accomplishments. More-recent continuation decisions are better documented. Both university and laboratory activities would benefit from standardization.

Under program-evaluation mechanisms, the COV noted that contractor meetings and workshops are extremely valuable for evaluation and mission issues. BES should consider expanding such meetings to more programs and it should invite some unfunded and/or young scientists to help bring new blood into programs. A supplementary mail review of laboratory site visits would be useful in some cases. An effective information-management system could be invaluable to staff in assisting the selection of the best program reviewers

Under program quality, the COV noted that top DOE research programs *are* world-class, competitive, and outstanding in any environment. For some areas, increasing the grant size at the

expense of programs at the decision margin might well produce better science for DOE. This is a complex area, because programmatic relevance is not a simple binary choice, as the COV has assumed. New initiatives can invigorate programs, especially when they can assist the core programs. New programs in AMO and nanoscience are clear examples.

Under staffing and program support, the COV concluded that the current SC information-management system needs to be replaced. It fails to provide the needed reviewer data about selection, frequency of usage, responsiveness, and quality of judgments. It fails to provide current or historical program support data in searchable, analyzable forms, and it forces program officers to develop parallel systems to track such information, producing a drag on the time of the professional staff. This situation makes it very difficult for program rotators to take advantage of prior experience, contributing to referee-selection issues. The staff is already very overworked, and adding new reporting responsibilities is not helpful. There is an urgent need to fill BES staff vacancies and to find ways to recruit new rotators and mechanisms that will allow them to function effectively in their new environment.

The COV process itself is viewed as informative and useful and should be continued if DOE can use the COV views. The process provides a GPRA-like [Government Performance and Results Act] overview of programs. The next COV will benefit from the experiences of this first round. The materials provided should be better focused on the Committee's task, and visitors should receive prior any COV report and BES responses. The COV would likely benefit most other areas in DOE.

The COV then offered a series of program-specific recommendations:

AMO Physics and Chemical Physics are very strong, active, well-managed programs. The science they produce is viewed as first rate. They have a significant number of new investigators and programs; the DOE-sponsored AMO workshop in 1997, together with new initiatives, has produced dramatic improvement.

Chemical Engineering is a small program with some strong projects. Its activities are narrow compared with the program name. Both new starts and turnover are extremely low. Perhaps it would be better to incorporate this small program into one or more larger BES programs.

Photochemistry and Radiation Science is a very strong, well-managed program with first-rate science. It benefits from very high-quality, thoughtful proposal reviews and very successful annual contractor meetings.

In Separations and Analysis, the top programs are outstanding, and the program is well managed. Possibly better science would result from increasing some of the best programs with funds from programs at the margin.

The Electrochemistry program is a fairly small program, but one that is a very important basic/applied program area for BES. It needs strengthening on fundamental aspects of the field. Some broadly based regular workshops with outside participation could expand the program's vision, as occurred with AMO. Funding-decision documentation needs to more clearly address the basis for actions taken.

Heavy Element Chemistry is another relatively small program, but one that is very important for DOE programs. There is a small number of investigators in field, and they would benefit from regular workshops.

Catalysis and Chemical Transformations has a very good balance of programs; it is strong, healthy, and well managed

The COV appreciated this opportunity to work with BES leadership in this first external review

of their procedures. The members learned an enormous amount and believe that all mission-driven science programs would benefit tremendously from such open evaluation.

Crow asked what percent of the upper staff of BES is rotators, and what their average term is. Dehmer responded that 6 or 7 out of 35 or 36 program managers are rotators and that their term of 1 to 2 years is closely regulated by legislation.

Crow asked if proposal submission should be standardized. Lineberger said that the COV did not look at proposal formats or at deadlines. A standard seems to be evolving.

Richards commented that a disconnect exists between what BES does and what the budget people want. Expert reviews play a very important role, and the COV process meshes very nicely with the recommendations of the GPRA subpanel.

Plummer suggested that BESAC should set up a group to help the COV and BES in setting up standardized documentation and forms. Also, the nomination and selection process for choosing DOE award winners is not documented and is inconsistent.

Greene pointed out that curiosity-driven research was only vaguely mentioned in the presentation and should be delineated more forcefully in the final report. Lineberger said that some hard facts will appear in the final report, but there are issues of privacy. The charge of the COV was to identify problem areas not to provide solutions.

Lester noted that each group worked at a very detailed level, particularly at the decision margins, but the report lacks the details that the groups saw. BESAC can set the level of detail that is finally reported. That is a delicate issue.

Kohn agreed with the recommendation of standardization, but added that it is also important to encourage people to go beyond standard requirements. It is a subtle business and difficult to prejudge what is going to be important. Lineberger responded that the COV was interested in the historic process and was looking for specific events in each case; these cases need to be laid out in a logical way so they can be found retrospectively.

Tromp asked if there was an industrial component of all this that had not been picked up. Lineberger answered that the major industrial activity involves the user facilities, which the COV did not look at. Dehmer added that those activities are managed by the facility managers themselves; those activities do not go through headquarters.

Shen asked about accomplishment-based activities. Lineberger responded that the NSF model of COVs allows consideration of both accomplishment- and proposal-based activities. But here the difference is between national laboratories and universities. The university proposals are small and narrowly defined; the laboratory proposals are larger and more highly aggregated and integrated; that makes it difficult to judge on an individual-accomplishment basis.

Johnson asked if the COV assessed the risk involved in proposed projects. Lineberger said that the percent of renewal is fairly high; they are long-term programs. The COV saw turnover rates from large to very low. It saw no clear evidence that bringing in new people was lacking. When new initiatives appeared, new people and activities were supported.

Crow asked if the COV saw any areas where technology could significantly impact submission, review, and follow-up of proposals. Lineberger responded that a little appears about that subject in the full report; the COV's anecdotal evidence indicates that technology could be very useful, especially for retrospective analyses of quality of review, speediness of review, etc.

Mayes asked if data on new starts will be included in the full report. Lineberger said that he was not sure how much data exists on that topic. There was one program where the COV was struck by

the low turnover rate. Lester added that the COV only looked at a very small sampling of projects. It did not look at that problem intensively. DOE should be able to provide that data much more completely. The laboratory reviews are done differently and still have a way to go in developing the process.

Dehmer thanked the Committee for their work. In 1999, BES put in place a new way of doing the laboratory reviews, and additional changes are going to be made. She will pass along the additional recommendations and Ward Plummer's comment to the BES staff.

McCurdy asked if COVs are being started in other DOE offices. Dehmer replied that other offices are not considering establishing COVs but that BES intends to expand this throughout the Office and to establish it on a 3-year cycle.

Richmond proposed that she write to James Decker, expressing enthusiasm with the COV process and with the prospect of its being expanded.

Crow asked Dehmer to report back on these activities at the September meeting.

Richmond introduced **John Stringer** to report on the Subpanel on Performance Measurement in the Office of Science. Stringer reviewed the makeup of the subpanel and its charge: to review (1) the Office of Science's methods for performance measurement, (2) the appropriateness and comprehensiveness of the methods, (3) the effects on science programs, and (4) SC's integration of performance measures with the budget process as required by the Government Performance and Results Act (GPRA). He pointed out that what was asked for in the charge was not what was what was really needed or wanted and that the time for preparing the report was very short.

The original overall objective of GPRA was "to provide for the establishment of strategic planning and performance measurement in the Federal Government." One of its purposes was to "initiate program performance reform with a series of pilot projects in setting program goals, measuring program performance against these goals, and reporting publicly on their progress." Strategic plans were called for: "No later than September 30, 1997, the head of each agency shall submit to the Director of the Office of Management and Budget and to the Congress a strategic plan for program activities. The strategic plan shall cover a period of not less than five years forward from the fiscal year in which it is submitted, and shall be updated and revised at least every three years."

The processes of assessment must be flexible and allow for information produced in the course of a project to alter the course of that project. That is why a strategic plan is so important.

The Act also modifies earlier legislation concerning performance plans, to begin with fiscal year 1999, and states that: "the Director of the Office of Management and Budget shall require each agency to prepare an annual performance plan covering each program activity set forth in the budget of such agency." The strategic plan must be related to the budget development and must "establish performance goals to define the level of performance to be achieved by a program activity" and "express such goals in an objective, quantifiable, and measurable form unless authorized to be in an alternative form." Such an alternative form may be authorized by the Director of the Office of Management and Budget. The Act allows an agency to "aggregate, disaggregate, or consolidate program activities, except that any aggregation or consolidation may not omit or minimize the significance of any program activity constituting a major function or operation for the agency." It requires that "no later than March 31, 2000, and no later than March 31 of each year thereafter, the head of each agency shall prepare and submit to the President and the Congress, a report on program performance for the previous fiscal year."

The Committee on Science, Engineering, and Public Policy (COSEPUP) noted that "It became

clear, however, that substantial problems existed for agencies trying to evaluate basic research programs. Urgent concern was expressed that basic research could not be effectively evaluated in the context of GPRA and that misguided attempts to do so could cause great damage."

The subpanel recommends that

1. The Office of Science complete its Strategic Plan as soon as possible.
2. The Office of Science continue to follow the general principles of performance assessment it has used in the past, including the use of COVs and other expert reviews.
3. The Office of Science's performance-measurement criteria be aligned with those that have been developed by COSEPUP (and with their ongoing studies on the development of criteria for basic research) to allow a common basis for the different federal agencies that support basic research programs, especially in the use of terminology.
4. The discussions between the Office of Science and the Office of Management and Budget regarding appropriate criteria for the assessment of the progress of basic science programs be continued in order to allow the development of appropriate metrics.

All parties involved agree that these actions (1) are necessary, (2) are probably good, and (3) should be done well and not harm American science.

In addition, the subpanel found that DOE's Strategic Plan and budget documents have to be framed in language that allows various readerships to understand the complexity and the extent of the Office's activities. Moreover, the Subpanel believes that the writing of a new Strategic Plan is a matter of great importance, and the Office needs to start the planning process as soon as possible. The Subpanel was told by the Office of Science staff that development of a new Plan is already under way, but it appears that there has been little formal involvement of the stakeholders. Moreover, the COSEPUP reports have reaffirmed the principle that performance of research programs should be assessed in terms of (1) quality, (2) relevance, and (3) leadership. This has been the objective of the Office of Science for many years, but the new role of assessment in the budgetary structure means that the meanings of these terms (and the ways in which they are assessed) have to be reexamined. In the view of the Subcommittee, the methods currently being used by the Office to measure quality are appropriate and adequate and should continue to be used. It notes, however, that relevance must relate to the mission of the agency as well as to the possibility of contributing to the advance of a discipline.

Other recommendations of the Subcommittee are that

5. Criteria should be developed to assess the "world leadership" element of the Office of Science's research and
6. Work-force issues, including the development of succession plans for the research staffs and the education and training of a technically sophisticated personnel reservoir for the future of the nation, be incorporated into the GPRA goals of the Office of Science.

A final finding was that much basic research is better assessed in qualitative terms. While this approach offers challenges to the concept of being "measurable," it should not lead to the imposition of quantitative goals. To do so would have significant negative effects on basic research and would certainly not be consistent with the principle that the application of GPRA should "do no harm," a principle agreed to by all the participants in this exercise. In DOE's ongoing discussions with OMB, this issue should be reviewed..

This topic must be dealt with; the problem will not go away. GPRA will help SC a lot, so SC should develop performance measurements as best it can.

Richards added that it is easy to trivialize what is very important. The Subcommittee encourages that the full value of the SC program not be trivialized by making just a minimal response to the GPRA requirements. OMB, Congress, DOE, and the public must be educated in performance measurement. Gilman, who sat on the Subcommittee, pointed out that there are tremendous dangers in trying to quantitate things that cannot be quantified. There is, however, an opportunity here to show the relevance and benefits of DOE's research. Sauthoff, another member of the Subcommittee, noted that one has to be careful that the Office's budget documents not be representative because they can easily be misinterpreted. We must describe programs and annual goals in a way they can be measured. That is a real challenge.

McCurdy asked what the relationship is among all the planning exercises that have been carried out in the past several years. Dehmer answered that each office must have a new strategic plan in place by September of this year. The previous strategic plans frequently responded to new administrations. That is often the driver for a new strategic plan.

Eugene Bierly commented that Recommendation 6 is there because it is linked with human resources, which goes beyond the language of the charge. The COSEPUP report calls attention to human resources, and DOE should give some attention to it, also.

A break for lunch was declared at 12:22 p.m. Richmond called the meeting back into session at 1:32 p.m. and introduced **Mark Alper** to report on the Biomolecular Materials Workshop, held January 13-14, 2002, in San Diego to identify specific research activities and goals and the nature of research in biomaterials. He defined *biomaterials* as materials, of any origin, designed for use as implanted medical devices or prostheses and *biomolecular/biomimetic materials* as materials designed for non-medical applications, whose structure or synthesis is derived from or is inspired by biology. The DOE mission does not include biomaterials research; that is supported by the National Institutes of Health (NIH) for biomedical applications. But NIH does not support some aspects of biomedical research (e.g., instrumentation). The DOE program could support spin-offs into biomedicine of materials and chemical-sciences research on instrumentation development.

Biomolecular materials are made by living organisms, made by living organisms and then modified in the laboratory, made by living organisms that have themselves been modified, made in vitro by a process that is unique to a living organism, or made in vitro by a process patterned after that employed by a living organism. Biomolecular materials use molecules, structures, processes, and/or concepts of biological systems as the basis for novel materials and devices to be used outside of living systems.

The properties, functions, and structures in living organisms are seen as attractive for nonbiological applications because they control structure at the atomic level, adapt to the environment, amplify signals, employ benign processing conditions, provide interfaces between living and nonliving materials, and employ biodegradable materials. They also control color, catalyze chemical reactions, perform combinatorial syntheses, convert energy, evolve, withstand extreme environments, and employ hierarchical construction. They can be used to produce lightweight materials, lubricants, machines (motors, rotors, pumps, transporters, tractors, springs, and ratchets), materials by design , membranes, molecule-recognizing sensors, multifunctional materials, and nanoscale synthesis and function. Some of those functions are optical transmission, self-assembly, self-healing, sensing, structural components, templated synthesis, and transport.

Biologists and others have developed the tools to understand and manipulate biological structures and processes and to mimic biological concepts. Bone, teeth, eggshells, and enzymes have been

studied for decades to use them or their mimics in nonbiological applications. The workshop conclusion that it is now not only appropriate but important to support research in biomolecular materials for nonbiomedical applications

In many areas of materials research, a particular combination of elements, processed in a specific manner, has been shown by experiment or theory to have important properties. The focus of research then shifts to understanding why those properties arise and identifying altered compositions or processing conditions to enhance them further. In biomolecular materials research, the ideal already exists: an existing material, with its given properties, being used in a nonbiological environment. But biological systems are extremely complex. In many cases, it is not even known what molecules are involved in achieving a property or what their structure is. In reality, far less is known about these molecules and processes than about semiconductors, metals, and ceramics. As a result, applications of biomolecular materials lag far behind those of conventional materials. If one does not know what gives bone its exceptional properties, how can one construct something similar? The same is true for molecular motors and protein folding.

At least until now, research into, for example, the mechanism of myosin action, the basis for the development of nanomachines, was regarded as biomedical (and assigned to NIH) while research into the mechanism of superconductivity, required for the development of room-temperature superconductors, was regarded as materials science. The workshop concluded that basic research in biology, where it is not unreasonable to expect that the resulting understand will be critical to our learning to manipulate these systems for nonmedical applications, must be regarded as a legitimate area for DOE-BES support.

Biology is not like high-Tc superconductivity. It is like physics: a large collection of very different research topics unified, to some extent, by a common culture, way of thinking, or research approach. But few of these topics are sufficiently mature to allow a reasonable argument that material production is in the wings.

The workshop concluded that a research portfolio in biomolecular materials must be broad, and project selection should be based primarily on individual scientific merit; picking applications winners now is impossible. At the same time, the research portfolio in biomolecular materials must be sufficiently narrow that a critical mass for collaboration and interaction is created.

Barriers to developing a successful program include the facts that (1) physical scientists do not know biology, (2) biologists do not know of applications beyond pharmaceuticals and biomaterials, and (3) few collaborations between biology and the physical sciences have existed except for the application of instruments to the study of biology. The workshop concluded that a new generation of multidisciplinary students needs to be trained. Research proposals that are supported should support the training of students as well as demonstrate the participation of experts in both the relevant materials/chemistry and the biology.

The top future opportunities at the interface between the biological and physical sciences were seen to be self- and templated assembly and biomimetics, biomolecular functional systems (e.g., motors, rotors, tractors, catalysts, energy transducers, and gates and transporters), cell engineering and cells in artificial environments, and biomolecular functional systems. Some of the areas envisioned being addressed are (1) enzyme catalysis and the fine-tuning of enzymes to perform specific functions, (2) producing nonbiological enzymes, (3) flagellant motors, (4) kinesin as a tractor, and (5) photosynthetic mimicry.

Crow asked about the separation of biomaterials and bioscience. Dehmer responded that one has

to take a broad view; one has to look at the goal of the research. If the goals are aligned with DOE's mission, DOE could pursue the research. Thomas noted that other interagency groups are also working on this.

Samuel Stupp continued the presentation. The science discussed at the workshop was terrific. Before the workshop the goals were to look at (1) opportunities in artificial systems, (2) using cells to make materials, (3) modification of cells, and (4) biomimetics. Basically, there were two discussion groups, one on self-assembly and templated assembly and biomimetics and one on cell engineering (changing a cell in abiotic ways) and how a cell behaved in an artificial environment.

Two main topics excited great interest: (1) functional organic, inorganic, and hybrid materials derived from biological synthons and (2) biomimetic structures that try to emulate what we see in biology, building them with biological or completely abiotic (synthetic) blocks. There was a lot if interest in DNA nanomaterials and in the idea of organizing inorganic particles making complex assemblies using base pairings of DNA. Other discussions involved bioengineered viruses as synthons to create materials or liquid crystals. These syntheses could be carried out through base pairing and branching. One could also use DNA-protein hybrid materials to carry out these syntheses. Another idea was the production of ordered particles with a valence, arranging, for example, silicon microspheres in an sp^3 configuration. DNA-base computation was discussed. These ideas represent a synthesis capability that we do not currently have.

The problem of protein folding is very difficult, but there are simpler tasks that we can undertake like investigating near-biological materials that are made from simple molecules. That procedure would form an intermediate level of biomimetics.

We do not know how to do these things, but biology knows how to do them. Bones produce nanocrystals with identical crystallographic orientations. Maybe some day, we will have bone-inspired hybrids for electronics, superconducting magnetics, etc. The fundamental ideas exist in biology, and that is why biomolecular materials is such an important field. The chemical modification of cells has been done. Chemical modification allows one to attach a cell to an artificial substrate and to do synthetic chemistry in a cell with a material. This is a powerful capability in such fields as sensor development. This is a field that needs to be supported because it will advance many areas of technology as well as medicine.

Kohn asked if it was a cultural problem that chemistry, physics, etc. start their inquiries in closed systems, but in biology one just does not start from such a defined point; biology has a very different culture. Stupp replied that, in biology, one does not know fundamentally how things work, but one gets hints.

Shen asked what would be learned from myosin action. Alper responded that the point being made here is that, until recently, one would not justify doing the basic biology within the DOE mission. If one needed that fundamental research to develop superconductivity magnets, one can conduct that research as part of the DOE mission.

Richmond introduced **William Kirchhoff** to discuss a forthcoming BESAC-sponsored workshop. The catalysis workshop is in its early planning stages. Its title is Nanoscale Science, Next Steps: Controlling Chemical Reactivity. It will be held May 14-16, 2002. The driver for the workshop is that we get approximately 85% of our energy from making and breaking chemical bonds, plus catalysis is needed for environmental cleanup.

The workshop will have plenary talks and breakout sessions on what we need to know to control chemical reactivity. What do we need to measure to characterize catalytically driven chemistry?

What do we need to know about the relationship between structure and function in catalytic reactions? How can we optimize the systems we select for study? What statistical or combinatorial approaches might offer new insights? What can heterogeneous and homogeneous catalysis and biocatalysis learn from each other? What is the right organizational structure that is required to address the major challenges in catalysis? How can new concepts in catalysis impact energy production and use? What are the top real-world challenges?

Morse commented that the control of structure in polymerization is another topic that might be considered.

Richards asked if this consideration goes back to 100 femtoseconds. Kirchhoff replied affirmatively. Richards asked if it would address combinatorial mutagenic processes. Again, Kirchhoff answered yes. Stupp said that he should consider a smaller meeting then, of 50 to 70 people. He would get more out of the participants and would be able to manage it more easily. Perhaps it should be broken up into smaller group discussions. Kirchhoff said that they would like to have cross-fertilization. The breakout sessions would be of a manageable size. Plummer suggested that they might have 200 to 300 people. ORNL had that big a session on the nanoscience center, and it worked very well. He cautioned that the organizers need to have the key industrial people involved from day 1 and the material-science people, as well.

Kohn noted that "nano" appeared only once in all the topics mentioned and asked whether nanoscience should play a larger role. Kirchhoff replied that all of these processes are going to occur at the nanoscale. The emphasis is on the molecular level.

Greene suggested that he talk to George Whiteside, who has pointed out that we are looking for the right singularities. Some overlap between disciplines needs to be found. One needs to know how to speak the different languages. Kirchhoff noted that it is often good to have a really good facilitator. Richmond commented that it would be good to match names to the breakout sessions. Kirchhoff said that he would love to have that; also, he would like to have feedback on the breakout groups themselves.

Dehmer asked that those suggestions be turned back to her on the following morning. She then asked **William McCurdy** to speak about the upcoming workshop on theory and modeling in nanoscience. He pointed out that $3.1 million had been put into the ASCR budget for computational nanoscience, so ASCR and BES are going to cosponsor the workshop. Ellen Stechel from the Advanced Scientific Computing Advisory Committee (ASCAC) will co-host a preliminary workshop in mid-April. Possible topics and questions include:

From the perspective of BES:

Structure and dynamics of/in nano objects

Structure and dynamics of biomolecular materials

Properties of nanocrystals, nanotubes, and other fundamental units

From the perspective of ASCR:

Role of modern applied mathematics

Role of computer science

Development and implementation of scalable algorithms

The preliminary workshop will be held in April, a report will be issued in June, the large workshop will be held in August, a joint funding opportunity in computational nanoscience will be available in November, and the first award in computational nanoscience will be made in April 2003. The objective of the workshops will be to identify new scientific opportunities and needed resources

to advance the frontiers of nanoscience through theory, modeling, and simulation. Some of the best topics are at the interface of hard and soft materials.

Upon questioning, Dehmer defined the contribution from BES to be at least equal to that from ASCR and noted that some of the topics listed are already in the core research program. She cautioned that we do not want to just relabel what we are doing now. BES needs direction on how to proceed in the next few months.

Tromp asked if the focus is going to be on numeric-intensive types of problems or on theory and modeling in general, some of which requires big computers and some of which does not. McCurdy replied that it cannot just be work that can be done only on very large computers.

Stupp asked if they were going to invite any token experimentalists. McCurdy responded, yes, we have to bring in a sense of reality.

Kohn noted that there is a trend to eliminate theory from the discussion of modeling. He believed that that was is a pity. He called attention to methods for electronic structure that scale linearly with the number of electrons. There are theorems that say that, for large enough systems, such methods must exist. He asked if such things would be considered in the workshop. McCurdy said that this was the type of question he hopes will come up.

A break was declared at 3:20 p.m. The meeting was called back into session at 3:43 p.m. with the introduction of **Thom Mason** to give an update on the SNS, which is in the throes of construction.

The SNS, an accelerator-based neutron source, will begin operation in 2006. At 1.4 MW it will be about 8 times as powerful as ISIS, the world's leading pulsed spallation source. The peak thermal neutron flux will be 50 to 100 times that of the Institute Laue Langevin (ILL), and the SNS will be the world's leading facility for neutron scattering. The front end will be delivered in June, and the Center for Nanophase Material Science has been added to the site.

At the moment, the FY 02 request of $291 million was fully funded; the FY 03 request is $225 million, as anticipated; the overall project design is 73% complete; the overall the project is 36% complete (through Dec. 2001) and within budget and schedule constraints ($1.4 billion and a June 2006 completion date); significant site construction activities are now under way; there is good progress on all of the technical components (front end, superconducting linac, ring, target, and instruments); we continue to have excellent environmental, safety, and health (ES&H) performance; and a recent Office of Science semiannual (Lehman) review went well with no action items cited other than the next review in May.

All five project-funded instruments have been baselined. The new Experimental Facilities Division Director is Ian Anderson (formerly of ILL). The piezoelectric tuners have been baselined to provide flexibility and insurance. The linac tunnel concrete was completed six weeks early. The target building foundation, ring tunnel foundation and general construction, central helium liquefier (CHL), electrical substation, klystron gallery, and central utility building are under way, and progress is good. Significant amounts of dollars are being awarded in procurements of technical systems, and the project is staying within 2% of the cost estimate. A new estimate to complete (ETC) has been conducted, and the baseline has been updated following completion of the review. A detailed installation plan has been developed, and the hand-off from partner laboratories is now in place as part of ETC. The project is on track for front-end commissioning in the fall of this year.

The cost baseline shows that the project still has $121 million for contingencies. A favorable price on the units for the superconducting linac has allowed an option for 24 additional high-beta cavities to get higher energy.

A target-system test was carried out at the LANL/WNR [Weapons Neutron Research] facility in December 2001. The mercury has been drained, and preparations have been made for shipment of the containers back to ORNL. The bulk shield liner is now onsite in Oak Ridge.

Twelve instruments have been approved by the Experimental Facility Advisory Committee (EFAC). Of these, seven have been funded:

High-resolution backscattering spectrometer
Wide-angle thermal chopper spectrometer
Extended Q-range small-angle diffractometer
Third-generation powder diffractometer
Vertical-surface reflectometer
Horizontal-surface reflectometer
Cold neutron chopper spectrometer

Five others are in "hunting" mode and should be funded soon:

Engineering materials diffractometer
Disordered materials diffractometer
High-pressure diffractometer
High-resolution thermal chopper spectrometer
Single-crystal diffractometer

About ten additional instrument concepts are under development for consideration by the EFAC. Initial tests of the Lexitek high-resolution scintillation detector prototype have been completed on the QENS (Quasielastic Neutron Spectrometer) Upgrade Instrument Prototype (QUIP) prototyping neutron beamline at the Intense Pulsed Neutron Source (IPNS).

Currently, two instrument development teams (IDTs) are funded with additional teams in various stages of maturity. A proposal to BES for a high-pressure diffractometer is imminent. A proposal for an engineering diffractometer has been submitted to the Canadian Foundation for Innovation (it also includes a second thermal chopper spectrometer). A German team is carrying out R&D for a spin-echo spectrometer. Guidelines governing IDTs have been issued, incorporating input from advisory committees, the user group executive, workshops, and user meetings. These guidelines are being used to implement memoranda of understanding (MOUs) with the two funded IDTs and will be used as templates for future proposed instruments.

A white paper has been drafted to describe the expected operational mode in the early years of operation following project completion (CD-4; 10^{13} protons delivered to the target, reflecting a functioning facility) incorporating operating budget plans and commissioning plans (starting this summer). The white paper is intended to stimulate discussion on the topic and, following dialog between accelerator/experimental systems and users (plus ASAC, EFAC, DOE, etc.), form a basis for (1) planning; (2) decisions on spares, designs, budget, etc. that impact reliability; and (3) setting user expectations. It breaks operations into 6-month segments following CD-4 with a goal to attain MW-class user mode after 2 years. User mode is defined by >90% reliability with respect to schedule with power level and availability (total number of hours) as variables to be maximized subject to that constraint. The white paper lays out possible paths to the ultimate goal of 95% reliability, 1.4 MW, and 5000 user hours per year. Once consultation is complete, the white paper will be issued to the community.

Crow asked if there are any discussions elsewhere on instruments that would compete with this. Mason said that the Japanese have proposed a 600-KW machine with add-ons for specific

capabilities (and a 2006 completion). The SNS is a dedicated facility and should get a better bang for the buck. The Europeans are pursuing a more ambitious facility but are having difficulty getting 12 countries to agree to it (a 2015 completion date is probably the earliest to be hoped for).

Greene noted that there are no muons, that you have to go to Switzerland or British Columbia to study them. Why not here? Mason said that, if there is additional science that can be done that does not compromise the facility's basic mission, we are willing to talk with anyone with the funding to do that research. We have not had any proposals from the muon community. Greene noted that some of the key people have moved out of the country. Mason went on to say that the SNS is not attractive to them because its pulses are too short for a continuous beam but too long for the muon lifetime.

Richmond introduced **Walter Stevens** to speak on basic research needs to counter terrorism.

Homeland defense and counter-terrorism may play a large role in upcoming budget requests. Of 13 or 14 homeland defense categories of focus, 6 map onto science:

Detection
Preparedness
Prevention
Protection
Incident management
Response and recovery

These terms should be the language used when science describes what it can do.

He quoted John Marberger's address to the AAAS meeting: "Science and engineering have critical roles to play in the war on terrorism. We need improved tools with which to prevent, detect, protect, and treat victims of chemical, biological, radiological, nuclear, and conventional terrorist attacks. Additionally, we will need new and improved tools to recover facilities from those same types of attacks, should they ever occur."

Combating terrorism will be a problem for many years to come. A workshop will be held to identify critical science issues and opportunities in research areas supported by BES that will be important to our nation's ability to detect, prevent, protect against, and respond to future terrorist threats. The expected outcome from the workshop is a report that will summarize the presentations and discussions and include recommendations for future basic research investment needs. The BES lead is Walter Stevens; the chairman is Terry Michalske, SNL; and the keynote speaker is Jay Davis, National Security Fellow, LLNL, and former Director, Defense Threat Reduction Agency.

The workshop will focus on the scientific issues underlying the detection, containment, sampling, analysis, decontamination, and destruction of chemical threats (including conventional explosives and toxic chemicals, such as choking agents, blood agents, blister agents, nerve agents, and by-products of their manufacture); biological threats (including bacteria, rickettsiae, viruses, fungi, and toxins, which, gram for gram, are much more deadly than chemical agents and can be bioengineered); and radiologic and nuclear threats (including nuclear explosives and radioactive materials and by-products of their manufacture).

The workshop will be held February 28 and March 1, 2002. The report will be posted on the BES website by the end of March. About 80 people are expected to attend. A survey of national laboratory research relevant to counter terrorism has been completed and will be included as an appendix to the report. Focused, individual workshops in the areas of chemical, biological, and nuclear/radiological threats are being considered for the summer 2002.

Moore asked why the program was strong on antipersonnel attacks but not on infrastructure

attacks. Stevens answered that not enough information had been found within BES to consider it. It is hoped that infrastructure threats and countermeasures will come out in the workshop. Moore asked what others are doing. Stevens replied that the Biological and Environmental Research Advisory Committee (BERAC) is also going to hold a workshop and that the defense portions of DOE have been working on this for a long time.

Dehmer commented that BES needs to have its goals understood by other portions of the research community. With the anthrax attack, a need was seen to revisit the Office's whole research portfolio. Stevens added that BES also needs to understand its role within DOE.

Richmond introduced **Iran Thomas** to speak on an upcoming BESAC-sponsored workshop on basic science needs for energy security. The workshop may be broken down into fossil, nuclear, renewable, hydrogen, fusion, electrical and consumption of energy, each with several subtopics. The first questions in each case are: Is there anything inherently wrong? Is it available? How long a supply is there? What alternatives are there? What basic research needs are there?

The offices of Nuclear Energy Research (NE), Fossil Energy (FE), and Energy Efficiency and Renewable Energy (EERE) are interested in the applied technology of those fields, not basic energy. One needs to ask if investment in basic research might pay off in significant contributions to the development of new commercial sources of energy. Once the workshop is held, it must be reported in a consistent style with consistent units. We are seeking people to help organize the workshop and people to participate in the workshop.

Tromp suggested that it might be best to pull out efficiency as a separate topic. Another issue that might be considered is the distribution of energy sources and availability, for example in wind energy. Thomas responded that a lot of information is available on distribution; the focus here is on basic research. We do not want to reinvent what already exists. Tromp said that he was not sure what Thomas meant by "basic." Something should not be excluded just because it is not potentially economically or sociologically interesting. Thomas replied that that is why wind, ocean, thermal, and other topics are on the agenda: to see if there is anything new that could be done.

Crow stated that deregulation is affecting transmission and networking and is affecting how utilities generate electricity. Thomas added that the same is true about cogeneration.

Moore asked about chemical storage. Thomas replied that, in the organization of the workshop, it would fall primarily under "storage" under "electrical energy." Morse noted that there are interesting features there for energy security. Thomas added that energy storage is also important for complementing many of the renewable sources.

Morse asked whether the title of the workshop refers to the military aspect of security. Thomas said, no, it is the strategic aspect. The United States has not been able to keep up with the growth of its economy by increasing efficiency; new sources of energy need to be looked at.

Dehmer commented that the goal is to look at this issue broadly in breakout groups that have to address all of these same topics and then pull their discussions together into a unified report that points to very obvious conclusions about sound investments that will lead to secure energy sources 10 to 20 years from now.

Mayes pointed out that the workshop is organized by production and consumption. One might want to divide each source by production, storage, transmission, etc. This is another way of slicing the pie. She asked whether people from materials science should be included to see where they can contribute to energy efficiency. Thomas stated that that level of detail is desired at the catalysis workshop but not so much here.

Kohn suggested that further development of sensors is needed. Thomas stated that sensors are extremely important in controlling manufacturing.

Kohn also suggested that the topics can be cut several ways. Mayes said that sensors could go under consumption; there are several issues involved with consumption.

Richmond asked that, during the coming evening, all Committee members consider potential candidates for populating the catalysis and energy workshops and that they report suggested participants to Dehmer the following morning.

Richmond opened the floor to public comment. Crow moved that the members of BESAC charge the Chair to express the Committee's collective gratitude to James Decker for his dedication and leadership as Acting Director of the Office of Science. Mayes seconded the motion, which was unanimously accepted.

Crow moved that the members of BESAC charge the Chair to express at an appropriate time the Committee's collective congratulations to Ray Orbach on his appointment and confirmation as Director of the Office of Science and to express the Committee's commitment to working with him and others in addressing issues and needs critical to DOE and the nation. Richards seconded the motion, which was unanimously accepted.

The meeting was opened up to other public comment. There being none, the meeting was adjourned for the day at 5:17 p.m.

Tuesday, February 26, 2002

Richmond called the meeting to order at 8:38 a.m. She asked for closure on the GPRA report. She moved to accept that Subpanel report. Richards seconded. The motion was passed unanimously. She took a straw poll on the completeness of the COV report. Several members wished to see a more complete draft before acting on it, so the final draft will be circulated, and an e-mail vote will be conducted on accepting it. She asked about the report of the Biomolecular Materials Workshop. Kohn pointed out that work done at LBNL needed to be included. Richards and Shen commented that the excitement and interest of the science presented were not reflected in the presentation, and they suggested waiting until the full report was available before acting on it.

Richmond brought up the topic of the Workshop on Basic Science Needs for Energy Security. Dehmer said that the current plan is preliminary and needs a lot of work to select and organize the topics, participants, and presentations. She needs feedback on what is missing from the outline and on people who should be included in the workshop. Alternate "cuts" of the subject matter might emerge during the planning process; that happened at the complex-systems workshop.

Mayes commented that the plan is quite comprehensive, although there is more to efficiency than just primary-fuel efficiency, and the treatment of the topic should be expanded. Thomas agreed and pointed out that end-use efficiencies feed back to the energy sources. Tromp pointed out that societal issues (environment, efficiency, etc.) could stand out in the list more prominently among all the technological issues. Kohn called attention to the workshop format and suggested that it use two "cuts"; the first day might consider the economic, environmental, etc. issues, and the second consider the issues related with the various energy sources. In wind energy, there are engineering challenges, but that is not what BES should be focusing on. Good judgment needs to be used in selecting how each topic should be approached.

Moore asked who in DOE pays attention to these larger issues. Singer said FE has looked at the

social effects of energy development; those types of concerns might be rolled into the "Issues" section of each topic in the outline. Moore voiced the concern that social sciences may have information needs based on the natural sciences. Thomas pointed to risk analysis as an example of the social sciences' overlapping with the natural sciences. That is not BES's forte, interest, or responsibility. Mitigation of the cause of concern, though, might be. Richards pointed to the differences in energy-production culture between the United States and France and said that such cultural aspects should be treated in the workshop.

Crow said that the goals of the workshop have to be more clearly defined. We need to look at, say, the materials and science issues that affect energy production and the more rapid implementation of new energy technologies. Stakeholders (utilities, consortia, etc.) should also be brought into the workshop and its planning process. Tromp pointed out the strong cultural component in play here. It might be good to bring in people from overseas to provide a different perspective. Thomas said that the best people on any subject need to be brought in wherever they come from.

Dove said that the issue of time scales needs to be addressed. Different scientific advances would have different time scales within which they would produce an effect. Some would be long term; others would be short term.

Mayes said that basic science needs should not be defined too narrowly. A mechanism needs to be includes for moving from science to practice. Thomas noted that there would be strong pressure for that from the technology side of DOE.

Kohn noted that nuclear energy at some time or other will play an important role in energy production in the United States. Safety and waste disposal are two areas in which basic science could make a contribution to the public use and acceptance of nuclear power.

Dove emphasized the role of the Earth sciences in this workshop.

Richmond called upon **Keith Hodgson** to present a brief update on the Linac Coherent Light Source (LCLS), a new facility engaging a broad range of experience and capabilities drawn from the synchrotron, laser, and high-energy-physics communities, providing x-ray photons in extremely short pulses and at extremely high brilliance.

Recent technical progress includes that on the photocathode gun. The performance of photocathode guns is a prime determinant of the output power in X-ray free-electron lasers (XFELs). The Gun Test Facility (GTF) at the Stanford Synchrotron Radiation Laboratory (SSRL) has demonstrated performance consistent with 0.6-μm-slice emittance at 0.2 nanocoulombs. These results, combined with computer models, produced a simulation that indicated that the GTF gun, providing this same beam to the LCLS, will produce a 140-fsec, 3- to 4-GW pulse at 1.5 Angstroms. This design, then, provides a good option for commissioning the LCLS with low charge and moderate power. (The LCLS design goal is 9 GW.)

At a January meeting of DOE-BES and SSRL/LCLS management, guidance was provided on the construction project's scope that excluded certain scientific instruments. This approach enables a more accurate definition of cost (experiments are more than 5 years away), of performance metrics for completion of construction project, and for flexibility in defining and funding the science program. The scope now being developed for the LCLS includes the facilities necessary to characterize the LCLS beam and to test the ability to filter, focus, synchronize with a pump laser, split/delay the x-ray beam for pump/probe experiments, and monochromatize. This then leads to developing a new strategy for the LCLS experimental program and the role of the LCLS Science Advisory Committee (SAC).

The schedule includes 2 years of project engineering and design (PED) prior to 3 years of construction, leading to operation in the fall of 2007. The PED funding proposed in the FY 03 budget request would begin work on engineering and detailed design. With design about 30% complete and successful validation and authorization from DOE construction review management, the next step would be construction. The total estimated cost (TEC) range is $165 to $225 million.

How to develop the experimental program needs to be considered. The LCLS SAC will be reformulated as an external advisory and oversight committee to consider proposals for LCLS instruments and science. The new SAC is being chaired by Prof. R. Falcone of UC Berkeley. The last meeting of the current SAC began to formulate a framework for the experimental program approach. The SAC strongly endorsed the principle of open, peer-reviewed access and competition based on science for decision making and operation in a general user (not a participating research team or collaborative access team) model, where SSRL coordinates activity (peer review) and technical management/general operation for scientific teams. The proposed framework and time line for the evolving LCLS science program would involve a call for letters of intent (LOIs) and R&D plans a few months from now, a planning workshop and call for proposals at the beginning of FY 03. Proposals would be reviewed and selectively approved in February of 2003. DOE would accept proposals for instruments a year later. Funding for three to five instruments would coincide with the beginning of construction at the beginning of FY 05.

Kohn said that he did not think that the scientific case was made for the LCLS at the previous meetings and that significant theoretical research could be done before the instruments are selected and installed and could contribute to guiding the scientific use of the facility. Hodgson replied that those comments were right on target and that the peer-review proposal process is where the guidance of such theoretical insight would be beneficial.

Johnson noted that 3-GW pulses were simulated for the photo cathode and asked where the technical hurdles were to reaching the 9-GW pulses projected for the photo cathode. Hodgson responded that the advances that have been made are relatively small but significant. Some improvements have been made in the simulated pulses. There will be a large worldwide effort brought to bear on this problem, and the modeling efforts show schemes that could produce tenths-of-femtosecond pulses, not just hundredths-of-femtosecond pulses and that would push the forefront of this machine.

Richmond introduced **Paul Lisowski** to present an update on the Los Alamos Neutron Science Center (LANSCE). The management of LANL and LANSCE are working very hard to follow the November 2000 BESAC review recommendations. Responsibility for overseeing the facility has been assigned to a single steward [the National Nuclear Security Administration (NNSA)], and an Executive Council has been established. An externally and internally peer-reviewed bottom-up cost estimate for LANSCE has been completed and reviewed by the Laboratory; all reviewers agreed on the costs to be borne. The ramp-up schedule was completed as part of the cost estimate. A funding increment of $10 million in the FY 03 LANSCE operations budget is planned. This process was begun with a successful CY 01 operating cycle, serving 270 user visits and 150 unique users. The goal to increase the LANSCE/Lujan user base to about 1000 users by 2006 is going to be a big stretch.

He reviewed the performance of LANSCE during 2001. For proton radiography, it provided 94% availability for 411 scheduled hours out of 466 total hours (20% more than scheduled); 100% beam delivery during dynamic shots; and a very successful experimental program with 36 shots. For

weapons neutron research, it provided 92% availability for 2501 scheduled hours. The Lujan Center provided 91% availability for 2734 scheduled hours; the beam downtimes of longer than 8 hours was outstanding at 1.7%; the beam current was limited to 55 μA because of target-moderator problems.

During the period, LANSCE commissioned five new scattering instruments and one nuclear science instrument: SMARTS, HIPPO, PROTEIN, PHAROS (rebuilt), ASTERIX, and DANCE. It developed and implemented a new generation of data-acquisition and chopper-control systems. The actinide basis for interim operations was approved by DOE, and LANSCE initiated plutonium experiments.

The 91.4% scheduled beam availability for the Lujan Center was unprecedented. It started at 75 μA and was intended to ramp up to 100 μA, but a cooling problem caused a cutback in operations to 50 μA. No equipment failures occurred for which the facility did not have spare parts, so downtime was very limited. A great variety of science was done by Lujan scientists this year. A Lujan scientist showed that protein structure can be solved by scattering from powders.

Major progress was made towards establishing a significant user base performing science at Lujan: 270 user visits were made by 150 unique users, and 113 unique experiments were run. Several hundreds of users are expected next year now that people know that schedules and machine availability are reliable. Performance in the 2001 run cycle was compared to that of the 1997 run cycle:

	1997	2001
Days delivered	85.8	104
Days scheduled	102.7	114
Users under age 40	50	74
Proposals run	136	113

The results of the 2001 User Satisfaction Survey were displayed and reflected overwhelming satisfaction with the operation of the facility by the users.

A well-planned outage started in December 2001, and the progress has been good. Work is now under way to replace the target moderator reflector system during the FY 02 outage. The neutronics design is complete, the mechanical design is substantially complete, and the procurements are under way. The user program is planned to restart on July 1; 6 months of beam delivery is planned to be offered this year. Beam delivery to the user facilities will be simplified by the installation of a switchyard kicker in the 2003 outage.

The 2002 LANSCE proposal cycle calendar calls for the call for proposals to be issued Feb. 4, proposals to be due Mar. 8, the Materials Program Advisory Committee to meet Apr. 22-23, the Nuclear Physics program Advisory Committee to meet Apr. 24-26, the schedule to be published on the Web June 1, and the user program to start July 1.

He summed up by noting that the priority for LANSCE within Los Alamos has been strongly supported by Los Alamos senior management. The LANSCE governance model is in place and working. With increased planning and a heroic effort from the staff, LANSCE has improved the reliability and carried out a successful scientific program. An annual outage is under way. No unexpected maintenance or repair issues have arisen to date. The Lujan target moderator reflector system replacement and switchyard kicker projects are under way. The proposal call is completed.

And the user program is scheduled for restart in July 2002.

Mayes congratulated Lisowski for the good performance of the facility. Greene also congratulated him on the turnaround.

Lisowski noted that they had seen a big growth in the university proposals. Plummer responded that that was great. However, money was provided for operating at 200 μA rather than 55 μA, and operation is at 30 Hz rather than 20 Hz, requiring other changes. Lisowski responded that LANSCE plans to go to 200 μA during the next two years.

Plummer asked if the California system is contributing the money for the LANSCE professorship and if the program is being expanded. Lisowski said that he believed that the program is successful and continuing to operate.

Kohn said that he would like to hear more about how these changes came about. Lisowski responded that LANSCE did not run well. The Plummer report enumerated the problems, and LANSCE was put in the deputy secretary's watch list. The confluence of these events led to the signing of a memorandum of understanding, assigning responsibility for operating the facility to NNSA. Second, we made a commitment to this Committee to work with DOE to establish a single steward for the facility. In a series of meetings of representatives of the sponsors and laboratory management, a memorandum of agreement was put together and signed by SC, Defense Programs (DP), and NE. That agreement defined how the facility was to be operated; it was based on the sponsor requirements and the potential of LANSCE.

Kohn asked how the interests of the scientific community will be protected in the future, given that the facility has been compromised in the past. Lisowski showed a series of quotations voicing commitment to the program by the Director of LANL, the Director of the Office of Defense Science, and the Los Alamos Senior Executive Team. He said that these statements, taken together, lend a lot of credence to the fact that LANSCE is going to be supporting science as a user facility.

Kohn asked him to put the scientific role of the facility in context with the Intense Pulsed Neutron Source (IPNS) and the ISIS research facility in England. Lisowski replied that IPNS has a very loyal user community. LANSCE will equal that user community in the next run cycle. But the quality of the instruments make a great difference. LANSCE has three world-class instruments that will make a difference to the science; it will eclipse IPNS with its higher power; and it will equal ISIS around 2006.

Richmond pointed out BESAC's critical role in improving LANSCE's performance. She asked for new business.

Plummer asked for a review of neutron facilities, specifically getting updates on the IPNS and the HFIR at the next meeting.

There being no other new business or any public comment, Richmond adjourned the meeting at 10:25 a.m.