Minutes for the
Basic Energy Sciences Advisory Committee Meeting
November 14-15, 2001,
Washingtonian Central Marriott Hotel, Gaithersburg, Maryland

BESAC members present:

Collin L. Broholm
Jack E. Crow
Laura H. Greene
Marsha I. Lester
Anne M. Mayes
C. Bradley Moore
John Richards
Zhi-Xun Shen
Joachim Stohr
Rudolf Tromp
Philip Bucksbaum
Mostafa A. El-Sayed, Vice Chair
Anthony M. Johnson
Gabrielle Long
C. William McCurdy, Jr.
Ward Plummer
Geraldine L. Richmond, Chair
Sunil Sinha
Samuel I. Stupp

BESAC members absent:

Patricia M. Dove
George Flynn
Walter Kohn
Cherry Murray
Kathleen C. Taylor
James A. Dumesic
D. Wayne Goodman
Daniel Morse
Richard E. Smalley

Also participating:

Paul Alivisatos, Director, Molecular Foundry, Lawrence Berkeley National Laboratory
Daniel Chemla, Director, Materials Science Division, Lawrence Berkeley National Laboratory
Scott Cram, Senior Science Advisor, Office of the Associate Laboratory Director, Los Alamos National Laboratory
Patricia Dehmer, Director, Office of Basic Energy Sciences, DOE
Jean Futrell, Director, Environmental Molecular Sciences Laboratory, Pacific Northwest National Laboratory
Linda Horton, Associate Division Director, Metals and Ceramics Division, Oak Ridge National Laboratory
Alan Hurd, Director, Manuel Lujan, Jr., Neutron Scattering Center, Los Alamos National Laboratory
Douglas Lowndes, Director, Center for Nanophase Materials Sciences, Oak Ridge National Laboratory
Thomas Meyer, Associate Laboratory Director, Strategic and Supporting Research Directorate, Los Alamos National Laboratory
Frederick O'Hara, BESAC Recording Secretary
James Roberto, Associate Director, Oak Ridge National Laboratory (Thursday only)
Iran Thomas, Associate Director, Office of Basic Energy Sciences; Director, Division of Materials Science, Office of Basic Energy Sciences, DOE

Wednesday, November 14

Chair Richmond called the meeting to order at 8:40 a.m. She welcomed the members and visitors. She said the main topic would be the science behind the Nanoscale Science Research Centers (NSRCs) and the Committee will be assessing each center separately. She asked each member to introduce himself or herself. After the introductions, Richmond introduced **Patricia Dehmer** to present the status of the Office of Basic Energy Science (BES).

The FY 2002 budget was signed by the President and for BES was within $1 million of the budget request ($1 million less for the NSRCs was appropriated than was asked for). The budget was larger than the previous year's because of the ramp-up in construction costs for the Spallation Neutron Source (SNS). The resulting total looks like an increase of $10 million, but it is actually a decrease because of the SBIR/STTR (Small Business Innovative Research/Small Business Technology Transfer Program) tax being subtracted. The good news is that there are no earmarks in the BES budget; the Office of Biological and Environmental Research (BER) budget had $72.1 million in earmarks for the Office of Science (SC).

John Marburger was confirmed as the head of the Office of Science and Technology Policy (OSTP). He made a speech in which he said: "We must make important choices together because we have neither unlimited resources, nor a monopoly of the world's scientific talent. ... We must still choose among the multitudes of possible research programs. We must decide which ones to launch, encourage, and enhance and which ones to modify, reevaluate, or redirect in keeping with our national needs and capabilities.

"Today the most pressing of these needs is an adequate and coordinated response to the vicious and destructive terrorist attacks on September 11, a response in which science and technology are already playing an important role. ... Two immense forces have emerged in recent decades to transform the way all science is performed, just as they have altered the conditions of our daily lives: access to powerful computing, and the technology of instrumentation which provides inexpensive means of sensing and analyzing our environment. These have opened entirely new horizons in every field of science from particle physics to medicine. Nanotechnology, for example, -- the ability to manipulate matter at the atomic and molecular level -- and molecular medicine the ability to tailor life essential substances atom by atom both owe their capabilities to advances in computing and instrumentation."

Secretary Abraham made a series of pertinent remarks at DOE's Quarterly Leadership Meeting. On management, he said that DOE should implement the kind of management changes that attract and retain the highest caliber people and DOE should expect to provide measurable performance objectives and accountability. On the Department's mission, DOE should identify new sources of energy for the future, protect our critical energy infrastructure, implement the President's energy plan, implement the President's climate change initiative, ensure the reliability of our stockpile, address the proliferation of nuclear weapons and technology, enhance homeland defense against new terrorist threats, and implement environmental cleanup faster and cheaper. He made special mention of two priorities. The first involves the unique technological contribution DOE can make to energy and national security by finding new sources of energy. We, as a nation, need to leapfrog the status quo and prepare for a future that, under any scenario, requires a revolution in how we find, produce, and deliver energy. The second is one that obviously flows from the tragic events of September 11, the challenge of responding to the threat of weapons of mass destruction posed by small groups of terrorists or by nation states.

The Secretary is very supportive of basic research, although that interest did not get emphasized in this speech. The Hart-Rudman report was very supportive of basic research and pointed out the need for that research in homeland security.

DOE's Office of Strategic Planning Activities has asked all elements of the Department to update their strategic plans, to link strategic planning with the budget process, and to articulate long-term goals and short-term targets by which progress can be measured.

- Macrotrends driving investment decisions by DOE, SC, and BES include
- Tool-driven science revolutions
- The increase in public demand for safe, reliable, efficient, environmentally responsible energy production and use
- National funding trends (e.g., those of the health and biological sciences)
- Evolving roles of national laboratory, university, and industrial research sectors
- International science, particularly the large projects

Major new tools have been developed or refined during the past 25 years, and BES has played a major role in several of these:

- Scattering; diffraction; imaging with electron beams, x-rays, and neutrons
- Lasers
- Probe microscopies
- High-speed, parallel processors
- Accelerator and detector technologies
- (Comparatively primitive) molecular-assembly and -disassembly techniques

The outcomes of these tools have been new knowledge, understanding, and control resulting from

- The visualization, understanding, and prediction of the atomic-scale assembly of materials of all kinds, from superconductors to genomes;
- Almost complete control and manipulation of materials at the mesoscale and microscale;
- Forays into the manipulation of materials at the atomic scale with man-made tools and Mother Nature's assembly tricks; and
- Fundamental structures of matter and their relation to the evolution and fate of the universe.

Subsequent revolutions include nanotechnology; biotechnology; computational modeling, a third branch of science complementing experiment and theory; and control of chemical reactivity to produce desired products with the absence of unwanted byproducts. These revolutions are a direct product of 25 years of investment in basic science. To reap the rewards of these revolutions, we will need to continue to invest in these tools.

Facility operations have increased from one-quarter to one-half of the work of the laboratories since the late eighties. That increase will continue in the future as investments in large facilities are made at the laboratories and they become centers of world-class research. University research is growing as well. These activities are resulting in the restoration of U.S. preeminence in neutron scattering and in continued U.S. preeminence in the sciences that use the facilities for x-ray diffraction, scattering, and imaging through the full utilization of existing facilities and the planning for the Linac Coherent Light Source.

Through the Nanoscale Science, Engineering, and Technology (NSET) university solicitation, BES plans to fund universities with up to $8 million for research. Preapplications are encouraged and are due November 16, 2001. Formal applications are due February 12, 2002. The NSET laboratory solicitation will provide up to $8 million for research. It is similar to last year's solicitation with the addition of the goal to attain an integrated structural and dynamic view of nanoassemblies in biological systems through the development of enhanced imaging tools and nanoscale probes. Proposals should be submitted through the field-work proposal (FWP) process.

To jumpstart the integration of nanoscience and biology, BES is holding a Nano/Bio Workshop on January 14-16, 2002, in La Jolla, California. Discussion topics will include:

- molecular interactions at the interface between biological and inorganic materials;
- the use of biological processes and molecules as synthetic tools for novel inorganic and organic nanomaterials;
- biomimetics of extracellular matrices, such as bone, cartilage, or enamel;
- the designed modification of cells and their interactions with their substrates; and
- the coupling of cells or biomolecules to photonic, electronic, and other devices.

The SNS is the largest federal science construction project. It recently had a week-long review, and the results were very complimentary. The project is on-time and within-budget and has experienced safe construction. (2002 is the main period of construction funding.) In 2002, DOE will restart the High-Flux Isotope Reactor (HFIR) and build up its user program. It anticipates the reliable operation of the Los Alamos Neutron Science Center (LANSCE), is going forward with instrumentation design and fabrication for the SNS, is working on the training of the next generation of scientists, and is participating in the Interagency Working Group on Neutron Science.

At the synchrotron light sources, the number of researchers using the synchrotron radiation light sources has gone from 1500 to 6500 in 10 years and is expected to reach about 11,000 annually when beamlines are fully instrumented. The goal is to make them reliable and easy to use for the research community.

The nationwide range of BES user facilities was reviewed.

The House Energy and Water Development Subcommittee has expressed concern that the Department does not have an adequate plan or policy that relates the basic research being conducted by the Office of Science to the energy needs of the country. The Subcommittee sees minimal cooperation and coordination between the Office of Science and other Departmental offices on the fundamental research needed to improve energy technologies. It has directed the Department to identify (1) ways in which coordination can be improved and (2) research conducted that is mutually beneficial and to report to the Committee by January 15, 2002. A letter of response will be drafted by a committee; BESAC will be asked for input.

Dehmer showed a table of about 100 DOE technology programs that indicated whether BES activities are highly supportive, moderately supportive, or nonsupportive of each program. The major finding was that BES contributes to all of those program areas in one way or another in renewable energy resources, nuclear energy, fossil energy, energy conservation, fusion-energy sciences, environmental management, nuclear-waste disposal, defense nuclear nonproliferation, and defense programs.

She reviewed the organization chart of the Office and pointed out that a number of vacancies exist. The Office now has approval to hire personnel for four positions, including that of Bob Marianelli, who is retiring.

James Decker has issued a new charge to BESAC, to lead a study to review SC's current method of performance measurement, an issue that involves all programs within SC, not just BES. To accomplish this task, BESAC is asked to assemble a subpanel to review:

- SC's current methods for performance measurement;
- The appropriateness and comprehensiveness of the methods;
- The effects on science programs; and
- SC's integration of performance measures with the budget process as required by the Government Performance and Results Act.

The subpanel will be comprised of one member from each SC advisory committee and two or three external participants with expertise in performance measurement. The activity will be limited to a 2-day meeting in the Washington area. A report to BESAC is planned for the February 25-26, 2002, meeting.

Future BESAC activities include

- Advisory Committee Review of SC Current Method of Performance Measurement, Washington, D.C., Winter 2001/2002
- Nano/Bio Workshop in La Jolla, California, January 14-16, 2002
- Committee of Visitors for Chemistry Programs at the Germantown DOE Complex, January 30-February 1, 2002
- BESAC full Committee Meeting at the Gaithersburg Marriott Washingtonian Center, February 25-26, 2002

In news from other agencies, the National Nuclear Security Administration (NNSA) is issuing a solicitation for a multiyear program at $10 to 15 million per year to fund centers of excellence, groups of investigators, and single investigators to conduct research in experimental science in support of stockpile stewardship. Information regarding this solicitation will be available on the Oakland Operations Office home page (www.oak.doe.gov).

Dehmer pointed out that BESAC members' comments from the August 2-3 BESAC meeting were organized into six areas and have been provided to the centers' directors in a summary outline:

- Science theme(s)
- Buildings, facilities, equipment, and instrumentation
- Management plan
- Laboratory and management and operating (M&O) contractor commitment
- Outreach
- Complementary activities

Those directors have prepared talks to address these issues at the current meeting. Dehmer asked BESAC for its view on how these projects are going forward. She reviewed the history of the NSRC program. These centers are new and different and are, therefore, undergoing numerous reviews and participation by the potential user research community. Based on the comments gathered at the prior meeting, a major part of the current meeting is devoted to lengthy presentations and discussions with the three centers that are moving forward with design: Lawrence Berkeley National Laboratory (LBNL), Oak Ridge National Laboratory (ORNL), and Los Alamos National Laboratory/Sandia National Laboratory (LANL/SNL). White papers addressing key issues were distributed to BESAC members electronically.

Stupp asked if there were gaps in the interagency coordination of the National Nanotechnology Initiative (NNI). Dehmer responded that the national laboratory initiative will continue. The Secretary and Marburger are supportive of the science involved. The extent of activity in the interagency working group is ongoing. She expressed a belief that there is good interagency coordination and cooperation. DOE SC asks its centers to report on their interaction with other agencies' activities.

Mayes expressed concern about the solicitations. The requests for proposals (RFPs) do not reflect the applicability to energy. How is the funding of these programs going to be reconciled with the Department's mission? Dehmer said that SC's activities will form around thematic areas that can be seen to relate to energy and to other agencies' research needs. Also, one needs to balance research directed at current mission needs with blue-sky research, where one does not know what will result. El-Sayed asked if the Committee could get a copy of these solicitations. Dehmer said, yes, they are available.

Richmond congratulated Dehmer on moving from being a highly regarded laboratory scientist to being a highly regarded administrator. She then asked **Z. X. Shen** about his meeting with Marburger. He said that the meeting was very productive. Several issues were brought up: (1) the scientific community's ability to respond to the events of September 11, (2) the balance of funding of science programs, and (3) the specific concern that there may be no new-start programs and how that might adversely affect the programs that support DOE's mission. Shen also met with Undersecretary Card and covered several of the same topics.

A break was declared at 9:57 a.m. The meeting was called back into session at 10:15 to hear **Paul Alivisatos** present an update on the Molecular Foundry, LBNL's NSRC.

The concept of a Molecular Foundry was developed over 3 years by a multidisciplinary group on what LBNL could do to influence material creation. It was designed to enable users to design, synthesize, and characterize state-of-the-art materials. Microlabs are limited in tools and techniques; this foundry will provide users rapid access to a variety of capabilities and the latest developments in materials creation. It will be a national user facility for research on nanoscale science and engineering, will provide a portal to the LBNL major nanoscale user facilities, and will provide the training and education of the "first" generation of nanoscale scientists. It is tied to the internal LBNL nanoscience research program.

Soft and hard matter often have different ways of patterning things and different ways to design materials: nanocrystals, nanorods, nanotubes, dendrimers, scanning-probe tips, patterned surfaces, cell membranes, DNA, and proteins. A user might be familiar with one of these ways; the Center will make all available and will give guidance on how to use them.

The Foundry will allow the addressing of important problems in nanoscience that require the use of multiple techniques for patterning and controlling matter. One example is the nanoscale design of energy-harvesting materials (e.g., nanorod-polymer photovoltaics).

An added value is the Center's enabling researchers to cover the entire "research cycle," including designing, synthesizing, measuring, analyzing, and returning to the design phase. This coverage of the entire cycle is the philosophical underpinning of the center.

The laboratory will be set up with seven subfacilities (with associated instrumentation):

- Inorganic Nanostructure Synthesis [chemical vapor deposition (CVD), molecular-beam epitaxy (MBE), laser ablation, and automated nanoscale synthesis],
- Nanofabrication (electron-beam lithography; microcontact/soft lithography),
- Organic Synthesis [nuclear magnetic resonance (NMR), electrospray-MALDI (matrix-assisted laser desorption/ionization)-mass spectrometry, spectroscopy/chromatography; peptides, DNA, carbohydrates, hybrids],
- Biopolymer Synthesis (NMR; electrospray-MALDI-mass spectrometry, spectroscopy/chromatography; peptides, DNA, carbohydrates, hybrids),
- Mammalian/Microbial/Plant Cell (a cell-culture facility; biohoods, incubators, microscopes and spectroscopy),
- Imaging/Characterization [scanning tunneling microscopy/atomic-force microscopy (STM/AFM), transmission electron microscopy (TEM), confocal microscopy, single-molecule fluorescence, focused ion beam, ultrahigh-resolution spectroscopy beamline facility], and
- Theory and Computation (Linux boxes).

Each subfacility will have state-of-the-art instrumentation; will be directed by senior Foundry investigators; will have a permanent, dedicated lead scientist; will include dedicated collaborative scientists and postdoctoral fellows; will have technical support staff; will conduct an internal research program to advance each area of fabrication; will have a budget for maintenance, upgrade, and replacement of equipment; and will be available to external users for no charge. The estimated facility staff will total 310.

Long asked what underlies the metric used here (the average user being expected to be onsite for 3 weeks). Alivisatos responded that those numbers were based on the recommended length of stay to bring a project to completion and the type of work being performed. Bucksbaum asked what fraction of these researchers would be short- and long-term users. Alivisatos said that three categories of users were envisioned. The first comes to the center, learns a technique, and goes home to use it; the second is a repetitive user of the center's unique capabilities; and the third wants to do something new that no one knows how to do yet.

Stupp noted that synthesizing a molecule is expensive research and that the logistics are complex. He asked how the Foundry fits in. Alivisatos that a user would come to the Foundry and someone with skills in that type of synthesis would help the user perform the desired activities. Each subfacility will have to struggle with how it makes that expertise available to the general public. Stupp commented that the amount of money needed to support such projects is huge. Thomas noted that the cost would be borne in several ways, including through LBNL's own research program and/or by other agencies. The cost to DOE will be that for the staff and instrumentation. The resources are not very large. Alivisatos commented that the point here is that the demand may be in excess of the resources available. Stupp said that it is the very complex problems that will be brought to such laboratories. Alivisatos offered the example of someone needing to make nanocrystals and being able to do it very well in one or two years at the researcher's home laboratory but being able to do it in a week or two at this specialized lab.

Sinha asked if three people will be able to handle 40 projects. Alivisatos said, yes. Some will be shorter term and some will be longer. There will also be the postdoctoral fellows who can help out.

Richards asked what portion might be repeat users. Thomas responded, about 15%. Tromp said that, with the cited ratio of staff, scientists would have to handle about one project a week; he asked if they would be swamped. Alivisatos said that one-third of a person's time would be used helping users do something that is already known (training them and then going on), one-third would be involved in helping long-term users, and one-third would be used to develop new capabilities. This way of doing it has not been done before.

The Foundry is modeled on the National Center for Electron Microscopy (NCEM) that hires outstanding postdoctoral fellows to collaborate with nonexpert users, allows users' projects to make the best use of forefront instruments and techniques, exposes the postdoctoral fellows to the wide breadth of problems brought to the center by users, and allows the postdoctoral fellows to pursue individual research projects. It is also modeled on the Advanced Light Source (ALS), where first-rate staff scientists provide high-level scientific collaboration with users who have the great ideas but limited experience in synchrotron-radiation instruments.

LBNL is already inundated with requests for collaboration with nanoscience researchers: Professor Ting Guo of the University of California, Davis, is currently learning to make cobalt nanocrystals and planning studies at the ALS; Dr. Natalia Zaitszeva of Lawrence Livermore National Laboratory (LLNL) has the goal of making silicon nanocrystal lasers; and Dr. Richard A. Vaia of the Air Force Research Laboratory (AFRL) at Wright-Patterson Air Force Base arranged a 3-week visit of a postdoctoral fellow to learn to make nanocrystals in support of polymer-nanocrystal-composite studies under way at AFRL. These people are being taught industrial techniques; the hope is that the Center will catalyze materials discovery by getting the users to use additional services.

Scientists at ALS are already performing photoelectron microscopy and nano research on indium wires that produce quantum-size effects. The electron-beam nanowriter is being used to make designer catalysts. The Foundry will enable rapid access to these and other user facilities at LBNL through the submission of an original proposal, by using director's discretionary time on instruments, or through a block of National Energy Research Scientific Computing Center (NERSC) time allocated to Foundry users.

The Molecular Foundry will be adjacent to the ALS, a 5-minute walk to the NCEM. The conceptual design report is 95% complete, and an advertisement for architect proposals was issued in October 2001. The start of construction is slated for 4Q, 2003. The building will have 52,900 sf. Other LBNL Facilities in proximity to the Foundry include the ALS, NCEM (which allows performing electron-optical techniques), and NERSC. NERSC has an outstanding independent research program and is listed number two on the Top 500 List of supercomputers worldwide. It has 4.5 TB of memory, 20 TB of shared parallel disk, and 35 TB total.

Several external advisory committees will guide operations. The Proposal Study Panel will have recognized scientists from the Foundry and other institutions who will review proposals based on IUPAP (International Union of Pure and Applied Physics) criteria. The Scientific Advisory Committee will oversee Foundry operation, policies, and their implementation; will advise on current operations, resource allocation, strategic planning, and budget development; and will review the direction of the facilities as the field evolves. The Executive User Committee will review user issues as they arise. The Molecular Foundry User Planning Committee will assist in determining the physical and organizational structure of the facilities during design and construction.

Reviews that the Foundry will undergo include a triennial LBNL Director's/University of California President's review, a triennial DOE/BES review, and ad hoc reviews.

It will conduct a lot of education and training in the form of short courses, summer schools, instrument-use courses, seminars, internships for undergraduates from disadvantaged local schools for technical positions, and an HBCU (Historically Black Colleges and Universities) summer program for promising undergraduates.

A workshop is scheduled for April 4-5, 2002, to inform the broad national community of plans to establish the Foundry and to solicit input on the design of the facilities.

Outstanding researchers will be attracted through a visiting scientist award, a distinguished investigator award, and graduate student awards.

The ratio of internal to external users will be determined by proposal competition with no guarantees for internal users. Less than 25% internal participation is expected.

Lester asked what he meant by external and internal. Alivisatos said that each facility will be charged with pushing the envelope and each will differ in how they do that. The object is to promote competition at the edge of scientific knowledge. Lester asked if there would be teams for focus areas. Alivisatos responded that there will be facility staff and users to collaborate. In addition, the Foundry hopes to cooperate with other BES NSRCs as well as with other nanoscience centers [e.g., the California Institutes for Science and Innovation, National Science Foundation (NSF) National Nanofab Facilities, NSF Nanoscale Science and Engineering Centers (NSECs), and other nanoscience research activities not necessarily associated with a center].

The Foundry has extremely strong support from C. V. Shank, the Laboratory's Director.

Crow asked him to comment on the level of access the users will have to other resources. Alivisatos said that NERSC has dedicated a block of time for the Foundry's users, and this is being used as a model for the use of the ALS and of other facilities. Crow asked if any thought had been given to performance measures for the facility in general. Alivisatos responded, no. Broholm suggested that, in producing functional devices, the ultimate measure is the marketplace: the number of applied devices produced, patents applied for, publications, etc.

Alivisatos assumed that the question of metrics would be the same for all user facilities. Dehmer noted that all BES user facilities have to report annually on a standard form.

Crow commented that, in the proposal portion, one sets milestones and deliverables. Those then get lost in the reporting process. Dehmer said that that accountability is exacted in the triennial reviews. Crow stated that, as proposals come in, the impact of previous proposals should be looked at.

Richards asked what was being done at the University of California at Santa Barbara (UCSB) and the University of California at Los Angeles (UCLA). Alivisatos said that that is a state institute dedicated to doing nanoscience; it is not a user facility.

Mayes asked what mechanism would be used to incorporate capabilities that were developed at other institutions. Alivisatos replied that LBNL would like those “artisans” to bring their expertise to the Foundry to allow their capabilities to be used more widely. Monies are available to bring in such experts to share their capabilities.

Shen asked how intellectual property will be dealt with; this will be a big issue in the community. Alivisatos acknowledged that this issue has not been thought through. The standard procedure is to grant intellectual property rights to the user, although sometimes it gets interesting with the involvement of the lawyers of the various institutions.

Broholm asked how much all of this will cost. Alivisatos said $85 million in construction. Crow asked if instruments were included in that sum. Alivisatos said that instruments would cost $20 to 25 million additional. Thomas commented that these figures are preliminary, unreviewed numbers that the Department has not agreed to.

El-Sayed asked if the center will be used for doing specialized measurements. Alivisatos responded that the issue of measurements has a lot of facilities devoted to it already. The Foundry will need measurement components, but that will not be the focus of the center; the focus will be fabrication.

Crow asked what money is available next year for these centers. Dehmer said $1 million will be available for each center in FY02 to cover preliminary design costs. What would be ideal would be engineering and design to be finished in FY03 and construction completed by FY05. Architect-engineer costs would not be finished until FY03.

Johnson noted that a postdoctoral fellowship is considered a major career step. It seems these postdoctoral fellows would bounce from project to project, leading to no publications. Alivisatos said that postdoctoral fellows are desirable because they will want to work on something that will lead to a job. They can root through the possibilities coming in and pick out the most interesting.

The meeting was adjourned for lunch at 11:49 a.m. It was called back into session at 1:15 p.m. to hear a presentation by **Douglas Lowndes** on the planned Center for Nanophase Materials Science (CNMS) at ORNL. Lowndes reviewed the membership of the CNMS development team and pointed out that the nanometer length scale is midway between the atomic scale and the submicron scale, and the greatest challenges and opportunities occur at the boundaries of academic disciplines. As a result, the current scientific infrastructure not well suited for research or education at the nanoscale. Resources need to be maximized, and multidisciplinary interactions need to be promoted to enable research of a scope and depth beyond current national capabilities. The intent is to understand nanoscale materials and phenomena, to assemble resources and create synergies that will rapidly advance the knowledge of nanoscale materials and phenomena, to identify ways to integrate uniquely nanoscale phenomena and properties with the micro- and macroscales, and to create an environment for multidisciplinary research and education.

ORNL is designing the CNMS to be collocated with the SNS and the Joint Institute for Neutron Sciences (JINS) on ORNL’s new campus. The CNMS will accelerate discovery in nanoscale science by integrating nanoscale science with three synergistic research needs: neutron science, synthesis science, and theory-modeling-simulation (TMS).

Neutron science represents an opportunity to assume world leadership with the unique capabilities of neutron scattering to understand nanoscale materials and processes. Synthesis science (science-driven synthesis) is an enabler of new generations of advanced materials through TMS, search and discovery, and new synthesis pathways. Through the Nanomaterials Theory Institute, TMS will stimulate U.S. leadership in the design of new nanomaterials, the investigation of new pathways for materials synthesis, and the understanding of nanoscale phenomena.

The research will be organized under three scientific thrusts: soft materials, complex nanophase materials systems, and TMS.

The Center is envisioned to be an 80,000-sq ft four-level building plus a Nanofabrication Research Laboratory (NRL). The Center will have wet and dry materials synthesis and characterization laboratories, office space for staff and visitors, a Nanomaterials Theory Institute [with laboratories to access terascale computing facilities and expertise at the ORNL Center for Computational Sciences (CCS)], the NRL [with clean and environmentally controlled rooms, electron microscopes, nanoscale patterning (electron-beam writer/lithography), and facilities for the manipulation and integration of soft and hard materials]; and high-resolution scanning probes.

The vision for Nanoscience Research and Education is a collaborative research center for the design, synthesis, characterization, and TMS of nanoscale materials, phenomena, and assemblies to provide scientists from throughout the United States with access to state-of-the-art facilities and expertise, anchored by nationally recognized core research staff drawn from ORNL, universities, and industry. The CNMS Postdoctoral Fellowships Program will provide a training ground for the nation’s future scientists and faculty. It will also provide CNMS scholarships (local-expense support to ensure access by qualified graduate students and postdoctoral fellows) and expert technical assistance, training, and scientific collaboration.

The major impacts will be increased and will accelerate fundamental understanding in the research areas: growth mechanisms, self-assembly, transfer and coupling across interfaces, collective phenomena in low dimensionality, and inorganic/organic/biological interfaces. Many fields will be affected (e.g., structural materials, highly specific sensors, functional materials, medicine, catalysis, energy generation and storage, nanomechanics, and vacuum nano-electronics).

CNMS will be the world leader in using neutron scattering to make broad classes of nanoscale phenomena accessible to fundamental study. Leadership in science-driven synthesis via synergy with TMS will accelerate both the discovery and the understanding of advanced materials. The Nanomaterials Theory Institute will be a world leader for designing new functional materials and for investigating pathways for nanomaterials synthesis. It will generally stimulate and support the understanding of nanoscale phenomena. The Nanofabrication Research Laboratory (facilities and expertise) will be used to understand and direct nanoscale self-assembly and will functionally integrate the use of soft and hard materials. CNMS will be a leading center for multidisiciplinary NSET research and education in the United States and certainly will be the intellectual and operational focal point for the southeastern United States.

Two key requirements for the CNMS are research staffing and educational outreach. The staffing and mode of operation will be flexible and multidisciplinary. There will be more than ten research focus areas, which will be highly collaborative. Core research staff will include 18 full-time equivalents (FTEs; long-term visitors, including young faculty members), sabbatical visitors, and direct release-time purchases. It will also have up to 36 postdoctoral fellows from universities and hundreds of graduate students and short-term visitors per year. From one-half to three-quarters of the FTEs will be from other institutions. The Center will also provide a highly qualified technical support staff. Scholarships will cover full-time local living expenses for 35 FTE graduate students and 35 FTE short-term visitors (estimated to number 300 to 750 per year).The major criterion for participation will be the quality and suitability of the science to be conducted. Approval by a Proposal Selection Committee will be required.

CNMS will provide support for 18 FTE postdoctoral scholars; 6 postdoctoral fellows will be hired fully by CNMS, and 24 will be hired jointly with collaborating groups.

He reviewed the organizational chart of the Center. The Center will have an advisory committee, and a series of proposal-selection committees will provide additional information. The Advisory Committee will have experts in the three scientific thrusts and nanofabrication research. Its responsibilities include (1) recommending research focus areas and priorities; (2) reviewing ongoing research and educational activities; and (3) recommending the discontinuation of a research focus area or scientific thrust. Nine Advisory Committee members (six internal and three external) are being proposed. The Advisory Committee will provide the Center with flexibility to evolve.

Access by visiting scientists will be through the peer-review proposal-selection committees, one for each scientific thrust. There should be a single application process that is internally coordinated with (e.g.) SNS and HFIR and that is internally coordinated with other ORNL research centers or user facilities.

The first CNMS planning workshop had 278 registered participants from 67 institutions. The purpose of the CNMS Planning Workshop was to engage the national and regional scientific community in planning the Center and its research. Most of the time was devoted to three rounds of breakout discussion sessions. The goals for the breakout sessions were to (1) identify candidate collaborative research focus areas with the most important challenges to scientific understanding and equipment needs with the most significant opportunities for new technology; (2) identify university and ORNL champions for research focus areas (potential lead scientists for collaborative research who will build teams for research in the Center's scientific thrust areas); (3) develop a desired CNMS mode of operation and identify the infrastructure and support needs; (4) design methods to access existing ORNL facilities and capabilities useful for nanoscience research; and (5) establish outreach to and collaborations with other BES NSRCs.

In the soft materials area, the workshop identified as promising research areas (1) synthetic polymers and bio-inspired materials; (2) systems dominated by organic-inorganic interconnections; (3) the interfacing of nanostructures to biological systems (from synthesis to signal transduction); and (4) electronics on a molecular scale. Looking at the first of these focus areas in detail, the participants identified several scientific grand challenges: (1) 3-D structures with tailored properties and/or functions and (2) controlled supramolecular assembly of macromolecules. Other challenges identified included hybrid macromolecular systems, the control of interfacial phenomena, scaling of structures and properties, the characterization of interfaces, and modeling structure and dynamics in condensed phases.

The workshop participants identified technological opportunities and selected champions for each area. The collaborators said that up to 20 other key national leaders in polymers and biomaterials should be invited into the discussion. Interaction should be established with other centers, including the National Institute of Standards and Technology (NIST), the Georgia Institute of Technology Nano Center, and the NSF Materials Research Science and Engineering Centers (MERSECs) in polymer and biomaterials.

Two proposals were received to work in TMS:

1. Virtual synthesis and nanomaterials design's scientific challenges: chemistry-structure-properties; thermodynamics vs kinetics; theory and simulation across multiple length scales; prediction of materials with exceptional characteristics; and narrowing the search (optimized selection of candidate materials and processes).
2. Theoretical nano-interface science's scientific challenges are theory and simulation across multiple length and time scales.

In complex hard materials, candidate research focus areas identified included (1) carbon-based nanostructures with scientific challenges of fundamentals of growth at the atomic level; the problem of large-scale production of nanotubes and how to functionalize them; (2) nanostructured magnetic materials; (3) nanoscale interface science with scientific challenges in understanding and exploiting the dominance of nanoparticle/grain properties by interfaces/grain boundaries; and (4) thermodynamics at the nanoscale.

The CNMS equipment needs were initially surveyed during proposal writing with input from 15 universities. Candidate research focus areas were also surveyed during the workshop. Breakout sessions on revolutionary instruments were asked, "What are we missing?" A prioritized selection is to be made in future planning workshops and follow-on sessions. ORNL NSET programs provided a resource of both equipment and expertise that will be selectively incorporated in CNMS but fully accessible for collaboration.

The most strongly expressed need was for a nanofabrication research capability within CNMS that will integrate soft- and hard-material approaches in the same structures and conduct research on directed self-assembly for nanofabrication and linking to the microscale. This laboratory will provide access to clean rooms, electron-beam lithography, high-resolution electron microscopy, various scanning probes, and specialized material-handling facilities. It is believed that by exploiting the extensive synthesis capabilities of the CNMS, the NRL can develop unique nanofabrication capabilities at the national level.

The CNMS will be the premier center in the world for nanoscience research using neutrons; the static/dynamic information produced will be complementary to other methods. Coordination with other BES NSRCs is under way. The Center's staff is actively exploring and developing collaborative research interactions with federal, state, and university centers.

The CNMS candidate research focus areas and mode of operation are highly synergistic with the research of university collaborators. CNMS will provide access to state-of-the-art capabilities and training for graduate students and postdoctoral scholars.

Stohr asked if University of Tennessee (UT) personnel would be considered internal or external users? Lowndes said that UT people would be considered as external unless they were affiliated with the Center or ORNL.

Richards asked if people would use both ORNL's facilities and those at Berkeley. Lowndes responded, yes, that is part of the complementarity of the laboratories. Richards went on to ask if the ORNL center would entertain joint proposals. Lowndes said, yes, but the mechanics have not been worked out yet. Linda Horton is working on a unified framework for all the resources of ORNL.

El-Sayed asked what type of budget ORNL would like to have for the Center. Lowndes replied, \$32 million for the building and \$30 million for equipment. El-Sayed asked what fraction of the annual budget that was. Lowndes replied that almost all of that amount goes to salaries; between one-half and three-quarters will go to visitors.

Crow asked how the instrument agenda can be coordinated with the SNS and HFIR. Lowndes responded that the leadership of the Center has been briefed on the SNS instrumentation. The SNS will have a wide range of and great capabilities in instrumentation, which will be enhanced by the presence of the Center. The efforts of the design teams are being highly coordinated. Also, the Center has to be operating about a year before the SNS.

Lester asked if neutrons are suitable for nanomaterial research. Lowndes replied that the peak intensity of the SNS enables a large class of experiments and the instruments will be the best in the world, raising the sensitivity up to 250 times and achieving a resolution of as little as 5 . This ability opens the way to investigate molecular-level structures. In addition, one can exploit a lot of neutron-scattering opportunities, such as small-angle neutron scattering (SANS), reflectometry, and hydrogen/deuterium (H/D) contrast.

Sinha asked how many users were expected per year. Lowndes said that 300 to 350 visits per year were expected, based on the expected level of support. Figures from other user facilities in Oak Ridge indicate 300 to 750 such users. In the past two weeks, a lot of calls have been received from researchers who were unable to attend the workshop, so the level of use may have been underestimated. Sinha asked if the Center will influence the usage of the SNS. Lowndes responded, yes, and this will help rejuvenate the neutron-scattering community in the United States. He asked **Ward Plummer** to talk about the role of synthesis in materials discovery.

The philosophical need in the scientific community for these centers is to incubate new ideas and to foster discovery. We need to relearn how to integrate systems, characteristics, modeling, and design. Basic energy science is at the forefront of an intellectual pursuit and technological frontier. The proof is in the Nobel prizes since 1970: two in the 1970s, four in the 1980s, and six in the 1990s, covering quantum Hall effects (1985, 1998), high-Tc superconductivity (1987), fullerenes (1996), integrated circuit (2000), and conducting polymers (2000). Future Nobel prizes might be for giant magnetoresistance and organic superconductors. The benefits of such research is typified by the IBM Travelstar disk, which can store 4.1 GB/in^2 and commands a $100 billion/year market today.

The CNMS philosophy is that whoever controls the materials controls the science and the technology. Currently, our experimental samples are coming from Japan and elsewhere. In the future, we hope that those materials come from a CNMS in the United States, produced by science-driven synthesis or technologically driven processing.

The Nanophase Materials Sciences Workshop identified a large number of scientific challenges and technological opportunities to be addressed. These lists are works in progress and are growing daily. The Center is coordinated with theorists, university centers, and government labs around the country.

Crow said that he would like to see a more complete discussion about the instruments selected. Plummer responded that, at the workshop, the researchers wanted the reflectometer online immediately. Crow said that that is one instrument and asked about the match between the range and growth in synthesis and the available instrumentation. Lowndes said that a breakout session was held on nanoscience and neutrons but that people left without a clear understanding of the interrelationship. A special workshop is probably needed on that topic.

Thomas asked if they had considered establishing instrument design teams. Lowndes responded, yes, but they will be called experiment design teams to give them wider latitude.

El-Sayed asked where ORNL stood in this field of synthesis. Lowndes replied that it has great strengths in a lot of young people and in its interactions with researchers in carbon nanotubes. ORNL’s polymer chemists, electronmicroscopists, etc. have a great capability to do the analyses needed. Also, in oxide ceramics’ synthesis, the Laboratory has a great capability.

Stupp commented that neutrons will be extremely useful in the later stages of the field. Lowndes followed up that Jim Ryan pointed out that creative synthesis will be needed to make use of neutron science. Broholm noted that one cannot overestimate the change in scope for neutron scattering experiments that will results from the greater intensity of the SNS.

Mayes asked what the projected annual operating budget is. Horton said, $15 to 16 million. Lowndes reiterated that one-half to three-quarters of that will go to support the outside visitors. Mayes asked how they counted users. Lowndes said they use the number of collaborators: about 500 per year plus 36 postdoctoral fellows and 30 appointments for long-term visitors.

A break was declared at 2:43 p.m. The meeting was called back into session at 3:15 p.m. to hear an update on the LANL/SNL Center for Integrated Nanotechnologies (CINT).

Terry Michalske began the presentation by pointing out that the focus of CINT is to integrate across length scales. Its objectives are to develop the scientific principles that govern the performance and integration of nanoscale materials and to provide a national resource for training a new generation of researchers in nanoscience and nanotechnology The capabilities of the Center build off the strength of LANL and SNL. The future is difficult to predict, so some errors will probably be made along the way.

This Center has four scientific thrusts: (1) nanophotonics/nanoelectronics, (2) complex functional materials, (3) nano-bio-micro interfaces, and (4) nanomechanics. What is exciting is designing these nanomaterials from the bottom up, not driven by expectations drawn from the macroscale.

The transport of information and materials across interfaces will be critical biological and nonbiological tools developed from theoretical approaches and by interdisciplinary teams. The vision for the environment of CINT is to explore the path from scientific discovery to the integration of nanostructures into the micro/macro world, starting with theory and experiment and proceeding through synthesis, processing, and performance to integration.

Building such an environment takes expert personnel, a place for those experts to work, and the tools they need. The Center will have a core facility and gateways to SNL and LANL to tap into the capabilities of the two national laboratories. The core facility will be built in Albuquerque. The Center will use an existing building for the CINT Gateway to Sandia and will combine existing space and new construction for he CINT Gateway to Los Alamos.

The core will be made up of about 50 to 70 scientists; 40 postdoctoral fellows; 40 students; and 100 university, industry, and laboratory researchers. The operations budget will be about $19 million. The Core Facility will be located outside Kirtland Air Force Base (KAFB) to ensure open access. It will have an Integration Laboratory (clean room), a Characterization Laboratory, a Synthesis Laboratory, a Theory Laboratory, and an interaction space (conference rooms and classrooms with video links).

The CINT gateways will be used to provide rapid access to laboratory assets. The Gateway to Sandia will be focused on nanomaterials and microfabrication. The Gateway at Los Alamos will focus on nanomaterials and biosciences. A small amount of construction will move bioscience into the main LANL campus.

CINT collaborations will attract students and visiting scholars (open to all universities), from undergraduate interns to postdoctoral fellows. For undergraduates, it will be largely a summer experience. Graduate research assistants (about 40), visiting students (short- and long-term), and CINT resident students will perform a majority of the thesis work at CINT. About 40 postdoctoral associates will participate in an internationally competitive program. Visiting scholars plus university, industry, laboratory scientists on short- and long-term visits will round out the staffing. The Combustion Research Facility (CRF) at SNL, Livermore, will be used as a model. It has a flexible environment with experts that can form project-specific teams.

The CINT collaborative-proposal process will include peer review and will range from short- to long-term collaborations and from one-on-one to multiple-investigator teams. The Senior Management Team will have an external advisory committee, and the Technical Steering

Committee will select research to be conducted and will provide advice to the Executive Committee.

Feedback plays a key role in planning. It will be derived from formal reviews, former-collaborator feedback, nanocenter partnerships, and planning workshops with very broad participation. Feedback to date has included the recommendations that student and postdoc support and mentoring be included, that no costs accrue to visitors, that communications receive priority, that a proactive role be adopted in defining the science, and that a broad spectrum of collaborators be included.

The next steps will include focused workshops to define the research and to develop communication links with other nanocenters and the establishment of “seed” CINT collaborations.

Plummer expressed concern about the use of government workers as mentors and whether the Center recognized what it means to mentor a student. Richards strongly disagreed, observing that some of the student mentors at JPL (Jet Propulsion Laboratory) are a lot better at mentoring than faculty members at the California Institute of Technology (himself included). Simmons expressed the concern that students might be sent someplace where they did not get any attention or guidance. Tom Meyer said that LANL has a lot of experience with this and that he feels very good about this part of the proposal.

El-Sayed asked if they will solicit proposals in specific areas or be open-ended. Michalske replied that the solicitations will probably be a mix.

Andy Shreeve picked up the CINT presentation, pointing out that these thrust areas are a snapshot of what is being done now. CINT hopes to integrate these areas and to open up new areas. It is building on the capabilities of the investigators now at the laboratories. It will also be hiring new staff members.

Examples of science going on now include understanding the behavior of DNA as a function of counter-ion valency. One effort that could build on this topic is polymer nanocomposites that use polyelectrolyte templates. An important aspect that will allow building on the capabilities of the laboratories is that of the gateways. The Gateway to LANL opens the way to efforts like the development of very large phage display methods.

The team is excited about the new scientific challenges that can be approached, such as the integration of biomolecular assemblies into complex functional materials, forming hybrid biometallic materials. On a different level, what biology teaches about materials can be investigated. Universal scaling laws are being found to cover 20 decades of size in transport networks etc. The CINT will allow probing the laws by which biological systems are put together, allowing one to learn how to build up new nanoscale materials with new functions and behavior.

Jerry Simmons continued the CINT presentation, saying that, in nanophotonics and nanoelectronics, the interest is in understanding electronic, magnetic, and optical phenomena at the nanoscale. Demonstration of a new control over wavefunctions, interactions, and the density of states is desired. In nanomechanics, understanding the mechanisms and limits of mechanical deformation, understanding energy transfer into and out of materials, and discovering unique mechanical properties occurring at the nanoscale are objectives. In quantum transport, one would like to pursue (1) the energy spectroscopy of interacting 1-D wires and (2) double-layer undoped heterostructure.

A collaboration among the National High Magnetic Field Laboratory (NHMFL) in Tallahassee, Princeton University, and SNL has been going on for a year or two. Sandia brought to the table high-mobility growth, state-of-the-art electron-beam writing, and reactive-ion-beam etching (RIBE). With these capabilities, one can perform experiments that cannot be done any other way. Other unique capabilities that are available at CINT include photonics, lattices and optical amplification, and lasing in nanocrystal quantum dot (NQD) solids. A future goal is to combine quantum dots and photonic structures/lattices.

These capabilities will allow CINT to provide the nanoscience community with a broad spectrum of capabilities, expertise, and ideas so it can create new science and new scientists.

Bucksbaum observed that this is not really a user facility and asked how it is going to work. Michalske said that collaborations will be the foundation of the work performed. Focused workshops would be a good way to identify topics for core proposals.

Richards commented that these ideas are fabulous and represent great opportunities.

Thomas stated that the review of the conceptual design will be in December.

El-Sayed asked what fraction of money will go to outside vs inside recipients. Michalske said about half will go outside for resources. El-Sayed asked who decides on what the director promotes. Michalske said that a program now in operation brings 3 laboratories and 50 companies together; it requires a real relationship to be built, as will the operation of the Center. Shen asked about the process for selecting projects. Michalske said that an advisory committee will review proposals. Shen also asked about clearances for foreign students. Michalske noted that the core facilities will be outside the restricted area.

Thomas asked how this proposal stands with the SNL and LANL directors. Michalske replied that both laboratories have significant investment in nanoscience and organizations pursuing nanoscience. It is a prominent research thrust of each laboratory. Meyer, speaking for LANL, said that nanoscience is a centerpiece for the future. Lowndes noted that Jim Roberto has said that nanoscience is the highest-level priority for new projects at ORNL, which has broad experience in nanoscience-related activities; in addition, the Laboratory’s institutional plan has identified several nanoscience areas for the pursuit of excellence.

Dehmer asked if the New Mexico team could expand on the gateway concept. Michalske responded that the gateways will allow access to complementary tools of the laboratories, and a modest facility will be constructed at each laboratory to make this possible.

McCurdy asked them to comment on the role of theory and models. Michalske said that science will not make progress without theory and models. Both laboratories have high competencies in this area. But theory needs to be integrated throughout the Center, not off in a corner by itself; it should be connected with the physical experimental tools.

Shen commented that he had learned a lot about the capabilities at SNL and LANL that he had not understood before.

Richmond asked if there were any areas that the Committee would like to see expanded on.

Richards said that he liked the biology presentations that go from the nano to the micro to the real world, where one can sense it. He would like to hear how that occurs in other fields than biology. Richmond asked ORNL and LBNL to address this topic.

El-Sayed said that what is important is how you are going to use nanostructures.

Crow observed that the connection to the private sector is important and that the committee had heard very little about that connection. He asked where the interfaces might occur, and how such interfaces can be promoted. Stupp said that, from the point of view of the NNI, some near-term successes are going to be needed, so private-sector interest is very important.

Broholm said that he would like to hear how these centers relate to energy and DOE’s mission. Mayes noted that, as reflected in the priorities, at the August BESAC meeting, a lot of sentiment was expressed that these centers need to have a clear relationship between their activities and the energy-technology mission of DOE. Thomas stated that some of the factors that are not understood are how important nanoscale behavior is to the nuclear-weapons program and the limitations in the science. Nanoscience has a lot to do with energy, and that is why this agency is so interested in nanoscience. McCurdy commented that that sounds like the NSF fundamental-science justification for funding nanoscience. Thomas responded that the NSF has a broad mission in science and education that DOE does not have. These centers are unlike the NSF's centers in that they are oriented toward the DOE mission. If one can synthesize, fabricate, and control single-domain magnetic motors, one can have a big impact on electrical conversion. Broholm asked where advances are needed in nanoscience that justify the DOE involvement. Lowndes responded that there is a BES study of nanoscience and that each chapter has a section at the end discussing the relevance to the DOE mission. That study is available on the Web.

Richmond suggested that each facility give a summary of their contribution to the energy mission, broadly defined. Richards commented that one of the glories of American science is that it does not put every science and investigator in a box and cut them off from everyone else, like the French do. [Chemla applauded.]

Crow noted that the Oak Ridge team mentioned leveraging the DOE investment and stated that he would like to have the other centers look at that process more closely.

Sinha commented that nanoscience has all sorts of implications beyond energy. BESAC should also be thinking about how the centers should respond to Secretary Abraham's call to be mission directed. Thomas said that the mission encompasses the environment, nonproliferation of nuclear weapons, energy security, and user facilities for the nation as a whole.

Richmond observed that some of the best people in the field seem to be taking on a lot of administrative duties and stated that she would like some assurance that these researchers are not deterred from their scientific interests. She asked the representatives for the three centers to address briefly each of the issues raised by the Committee in the next day's session.

She called upon **Sam Stupp** to comment on the Nano/Bio Workshop to be held January 14-16, 2002, in La Jolla, California. He said that the goal of the workshop is to examine opportunities for mining biology to learn about and build artificial systems, particularly at the nanoscale. Some of the topics that would likely be touched upon at the workshop are quantum dots in bacteria; chemistries and new physics for the hierarchical organization of nanostructures; and a fresh look at biokinetics that would include ideas for electronics and photonics from tissue structure and the consideration of bone, cementum, cartilage, enamel, muscle, neural networks, etc., which embody many complex phenomena.

The cochairs of the workshop are Mark Alper and Sam Stupp. About 18 invited speakers will make presentations.

Richmond reviewed the schedule for the following morning. She called for public comment.

Jean Futrell of Pacific Northwest National Laboratory's Environmental Molecular Sciences Laboratory (EMSL) said that the presentations were exciting and that the committee asked the right questions. His laboratory and the CRF are somewhat like the centers proposed here. EMSL just went through their three-year review, and he offered their experience in planning to aid the planning for the NSRCs. Motorola had placed two workers in EMSL; they filed more than 300 patents when they went back to their home institution.

There being no further public comments, the meeting was adjourned at 5:11 p.m.

Thursday, November 15

Chair Richmond called the meeting to order at 8:30 a.m. She asked Dehmer for clarification of the upcoming charge from James Decker.

Dehmer said that the House Appropriations Committee has asked for a report on coordination and interaction between SC and other offices of DOE. A small group from SC will answer that request listing (1) principles for interaction and coordination, (2) best practices from past experience, and (3) templates for routine interactions. One of these best practices will be holding topical workshops in areas of interest to several offices. All the topics for joint workshops are based on existing boundary conditions; none are outside the box. How would one come up with one that is outside those boundaries? BESAC needs to think about how to do just that. One way would be to have a workshop on workshop topics that would not normally be considered. Thomas pointed out that joint workshops and other joint activities are ongoing among divisions of DOE with mutual interests; for example, Jerry Smith is assessing the superconductivity program to see how it is progressing. Such activities constantly occur. There is funding for such a detailed workshop if BESAC called for one. Dehmer noted that Environmental Management expressed an interest in participating in this type of activity. For every activity BES has, there is a counterpart in the technology program; advisory committees can drive interactions among those portions of DOE.

Mayes asked if Dehmer wanted these workshop ideas before the next BESAC meeting. Dehmer responded, not necessarily and asked if the best way to identify five or six topics that would be appropriate to drive interactions between BES and other portions of DOE would be to hold a one-day workshop. Bucksbaum commented that an effort to find out what is going on in the technology offices so BES could respond to specific needs would be one type of activity, but thinking outside the box would be another. Dehmer said that the question is how this Committee can help integrate the activities of DOE. Stohr asked what the box is. Dehmer said that one would not attain that perspective by sitting around a table or even by bringing in directors, the Secretary, or their representatives. The Committee will need to decide the agenda: What is to be accomplished? What briefings are needed? What needs to be apprised? The white paper out of DOE will set forth principles of interaction and best practices, but it will not think outside the box. It will be tactful. We are not going to think outside the box for the near term (5 years) because technology does not evolve that quickly.

Greene asked if she was asking how to get more people talking together. Greene noted that the ICAM (Institute for Complex Adaptive Matter) from Los Alamos had a disaster; biologists just talked with biologists. What is needed is to see what is working and then to invite people that can work together. The cooperation has to come from inside. One has to realize where the overlaps are, and that is really hard. One way is to report what has worked in a given workplace.

Richards pointed out that the Nano/Bio workshop in January is integration across scientific disciplines. Dehwer said she wanted something closer to technology.

Tromb observed that the only way that works is to take people from the science side and move them into technology. Thomas noted that Linda Horton at ORNL heads up a program like that.

Dehmer said that BES has a responsibility to make future impacts on missions. Primarily in the laboratories, DOE has people that are funded by both science and technology offices. They understand why they are doing what they are doing. She noted that, if she were in industry, she would probably be moved around to get a variety of experiences and spread that experience around the institution.

Richmond said that the Committee would have a better understanding of the charge related to integrating activities by the February meeting.

Stohr commented that one could use “technology” in a narrow sense, related to the missions of DOE, such as environmental cleanup. Dehmer agreed.

Richmond called upon the three NSRCs to come forward to discuss the five points identified by the Committee the previous day:

1. How will nanoscience allow researchers to go from the nano to the micro to the real world in fields other than biology?

2. Where might the interfaces occur between these centers and the private sector, and how can they be promoted?
3. What contribution would each of these facilities make to the energy mission, broadly defined?
4. How would each center leverage the DOE investment?
5. How would the centers assure that the best people in the field are not deterred from their scientific interests by the assignment of a lot of administrative duties?

Daniel Chemla made the response from LBNL's Molecular Foundry. LBNL sees the relationship of nano to macro in terms of nanocrystals, nanotubes, and nanowires. They have been using enzymes as restriction and connection aids in the vertical and horizontal assembly of linking tiles to produce lattices. They have also used this spontaneous-assembly method to assemble ribbons of magnetic nanorods, vortex patterns of CdSe rods, and DNA-directed assemblies of 5-nm and 10-nm gold nanocrystals. However, a lot of research is needed to exploit this technique. This self assembly and organization of inorganic nanocrystals is the first step toward functional systems of nano building units.

Other potential research directions at the Molecular Foundry include progressing from photosynthesis to a photovoltaic cell by using (1) a DNA oligomer that has a light-harvesting dendrimer and an acceptor porphyrin, (2) an organic/inorganic linker, and (3) CdSe NanoXal "storage." Already, the Center for X-Ray Optics (CXRO) extreme ultraviolet (EUV) lithography program (the CXRO nanowriter) makes 20-nm gates.

LBNL has ongoing industrial collaborations with more than 14 private corporations (Intel, IBM, Advanced Micro Devices, Motorola, Seagate, Advanced Materials, Hewlett Packard, Dupont, Dow Chemical, Novartis, Exponent, Q-Dot, CibaVision, Shipley etc.), looking at, for example, fibroblast cells labeled with CdSe nanocrystals to make quantum dots.

In terms of leverage, an investment in the Molecular Foundry will provide facilities and expertise to at least 300 research groups (funded by all agencies) per year. This center will spare the expense and time of each group's setting up its own capability. In addition, the Foundry will disseminate know-how and state-of-the-art techniques to research institutions across the United States.

Richmond observed that the ORNL proposal shows they will bring peer-reviewed projects with their own funding into the center. That practice will help ensure that users will be knowledgeable. Tromp commented that delivering photons is different from delivering expertise to users. Having lots of users travel through the laboratory week in and week out is a recipe for disaster. The New Mexico proposal is more reasonable in working with a limited number of focused clients. This whole model should be rethought. Chemla responded that the users are coming in to use a state-of-the-art instrument so they can do world-class science with the help of a good technician. That is the goal. Tromp asked if DOE wanted to do state-of-the-art research or run-of-the-mill production. El-Sayed pointed out that these researchers are the best brains in the country. Chemla reminded them of the three classes of user. This is a new way to think about how we do research. It is too early to ask such detailed questions. If you had asked Shockley and Bardeen the goal of their research, they would not have said, "to make a transistor." Richmond said that Chemla is saying users will vary from state-of-the-art to training; this group is saying that the priority should be on the state-of-the-art users. Chemla pointed out that, at the same time, DOE wants to see how many users will be served.

Tromp referred to another research facility that had two centers, one in Berkeley and one in Arizona. The one in Arizona was aimed at developing new Electron Microscopy (EM) techniques and tools. NSF demanded they act as a user facility. In a few years they went out of business.

Thomas commented that he did not see the difference between the light sources and the NSRCs. Light sources can pump out photons and still fail. It is the intellectual driving force that makes the difference. If you do not have world-class researchers, you will not have a world-class facility or world-class research. On the other hand, there may be routine data that one user needs to support someone else's world-class research. We have to provide both. The range of activities mirrors the activities at other facilities.

Tromp said that it is a matter of emphasis. If one emphasizes world-class research, that is good. But it is different from emphasizing thousands of users going through the doors. Thomas said that DOE is not going to grade these facilities by the number of users they treat.

Shen offered the observation that a wide range of activities need to be considered. He would not want casual users to use a synchrotron frequently because so many things can go wrong with ongoing research. On the other hand, computing services can be partitioned and easily shared. Sinha noted that, if the investment in these centers is to pay off, they have to do excellent science, involving collaboration among excellent scientists in-house and from outside, and produce new types of materials and new discoveries. If one has an excellent group, they will acquire the tools they need and do as much in-house as possible. He did not see how this user mode will work. Chemla said that one important point is the multidisciplinary aspect of this research. Specialized equipment and expertise will be needed on a short-term basis. The cost issue will prevail in such a situation. Shen said that, if one has a regional facility, they will travel to it. Johnson noted that researchers at second- and third-tier universities, where some of our brightest new graduates end up, should have access to these world-class instruments and facilities. Richmond commented that that can be addressed at the review-panel level.

She introduced **Douglas Lowndes** to make the Oak Ridge NSRC response. As examples of connecting nanoscale science to real-world technologies, he offered:

- Polymers and block copolymers for directed self-assembly of nanomaterials to produce building blocks or templates for the formation of bulk materials. One can direct this bottom-up approach to directed self-assembly with electric fields.
- Thin-film oxide fuel cells with nanoscale functionality that use nanoscale solid oxides with improved conversion efficiency.
- Carbon nanotube arrays for massively parallel electron-beam lithography.

How to promote interactions with the private sector? (1) Hold nanoscience workshops. There is dramatic interest from the private sector. The ORNL workshop involved 10 private companies, including three venture-capital investment companies with about $100 million each. ORNL has a strong track record in technology transfer and CRADAs (cooperative research and development agreements) with industry. (2) Include industrial partners in research focus areas and have industry representatives on the advisory council.

Nanoscience has a broad range of applications for energy technology in

- Fuel cells (nanostructured ionic conductors)
- Catalysts (improved efficiency and selectivity)
- Clathrates (carbon sequestration and energy supply)
- Sensors (highly specific environmental sensors)
- Energy-transmission materials (next-generation superconductors)
- Materials with improved thermal conductivity, electrical conductivity, etc. for energy applications
- Structural materials (light-weight, high-strength nanocomposites)
- Energy storage (carbon-based nanostructures)
- Improved magnets (lighter-weight motors)

- Energy generation (nanostructured photovoltaics)
- Self-assembled ordered materials (membranes for separation)

CNMS collaborations will leverage the nanoscience investments of state and federal agencies and will support university collaborations.

How to protect our leading scientists from administration burdens? Hire excellent support staff; include dedicated administrative support for scientific staff; establish a deputy director position; protect scientific-thrust leaders; and focus top scientists on building, leading, and running world-class science programs and collaborations.

We are trying to design a center that will maximize resources and promote multidisciplinary interactions to enable research of a scope and depth beyond current national capabilities. How do we do that? By hiring 36 people jointly with university research groups. ORNL held a workshop and asked attendees to identify candidate collaborative opportunities. They came up with an impressive list of topics and participants.

Crow said that the young scientists early in their careers should get some support as well as people with external support. Lowndes responded that such people would be able to participate through the focus groups.

El-Sayed asked if these appointments are going to be competed. Lowndes said that the Center has to be set up first and the focus areas identified. Then advisory committee members will be nominated. That committee will recommend budget distributions.

McCurdy noted that the two models (user facility and research facility) are extremes of a spectrum. One cannot have a world-class user facility without world-class research. It was a radical failure of imagination that these centers could not combine both ends of the spectrum between a self-contained, pure research facility and a pure user facility. He endorsed the three-class-user model put forward in the LBNL presentation and said that BESAC should trust its colleagues to find the right balance. Richmond said that top-quality research is a priority, but that does not mean that second- and third-tier universities will be excluded. El-Sayed commented that the leaders constituted a good selection of people; they will do it right.

Andrew Shreeve (LANL) made the SNL/LANL response. The connection between CINT and the private sector is typified by the laboratories' experience with successful technology-transfer partnerships, including the control and value of intellectual property. They currently have active collaborations in nanoscience with more than 8 companies and are promoting new connections with 14 other companies. They plan to include industry partners in workshops and advisory committees.

Nanoscience will contribute to DOE mission needs in energy security (e.g., solid-state lighting, long-term alternative energy, and energy efficiency), national security and nonproliferation (sensor development, diagnostics for material aging, and microdevice reliability), and environment (nanocluster-driven photocatalysis, interfacial science, and sensing and monitoring). It will provide scientific underpinnings that will lead to advances in all these mission areas.

Investments will be leveraged through partnerships funded by other government agencies (e.g., NSF), new joint proposals, application-oriented program development, long-term visiting by industry scientists, and funds in agreements and CRADAs.

Scientists will be protected from administrative demands by providing sufficient administrative and support staff [e.g., visitor interfaces; training; environment, safety, and health (ES&H); and collaborative user programs], adequate long-term technical support, and attractive CINT scientific staff positions (good career-growth and collaboration opportunities). The Center will learn from other user resources at the laboratories.

Mayes asked how CINT is going to interface with the Lujan Center. Alan Hurd of LANSCE said that they plan to create a proposal-review committee to allocate beam time and will ensure the availability of deuteration facilities. LANL scientists will be given discretionary time, including time on the new reflectometer. Mayes asked if time will be specifically set aside for CINT users. Hurd responded that beam allocation will be driven by the quality of the proposals.

Richmond called for general comments. Sinha asked rhetorically if this investment will make a huge difference in science in this country. He was sure it will. He asked if this center will function like a magnetic resonance spectroscopy (MRS) laboratory, where people can make use for their own purposes, or like a light source. He commented that the coupling of these centers with the ALS, SNS, HFIR, etc. will create a synergy that will be very productive.

Stohr asked what will precipitate the inclusion of additional NSRCs. Thomas responded that the other two laboratories are redoing their proposals and eventually will resubmit them. They will then be judged to see how good they are and how well they fit the current evolution of the facilities. Stohr asked what the review process will be like. Thomas said that he did not know yet. Greene stated that BESAC should play a role in that review process. Thomas said that he did not have any problem with that. The formality problem comes with the timing of the federal budget. Greene said that she believed that DOE should try to get all these centers funded and integrated. Dehmer said that Greene's point is appropriate. The current situation is different from that when the original solicitations went out, including an alteration of each of the three selected proposals by the suggestions of the Committee. Thomas noted that that is why the Committee had had these representatives before it so many times.

Moore commented that BESAC has to emphasize that this is a critical technological thrust for our country.

Shen asked if the Nano/Bio Workshop in January will introduce more activities in nanoscience. Dehmer responded, yes; we need to think beyond nano to bridging the nano and macro fields.

McCurdy observed that the work in nanoscience will likely revolutionize the theory as well as produce new materials and functionalities and that he was starting to see how theory and simulation will function as part of the nanoscience initiative. Thomas said that that point is important and will benefit the three centers. Dehmer said that she had definitely just heard McCurdy volunteer to lead a workshop on the topic.

Broholm submitted a written comment after the meeting for inclusion in the minutes:

All centers should be commended for their vigorous and imaginative efforts. I was impressed and I am enthusiastic about all of the proposed centers. I have general comments as well as specific comments for each of the centers. There are three general comments:

I think we all agree that the greatest potential for nano-scale science impact lies in the longer term. However, to be true to the vision of societal impact that was presented in the NNI, the nanoscience centers must remain engaged with industry. Centers should strive to keep potential industrial partners informed of novel processes and technologies so that these can be brought to the marketplace and to the consumer. Conversely, center scientists need to hear from industry about what their major problems are, not to provide government support for short-term research needs, but for inspiration to think about problems whose solutions could have a major societal impact. Scientists thrive on challenges, and my experience from two years at Bell Laboratories is that the challenges presented in modern technology are every bit as exciting and as important as the challenges of basic science.

The BES impact on science is and should be much greater than simply in energy technologies. However, the DOE nano-science centers have a special opportunity and obligation to harness nanoscience to address our pressing energy needs. I believe that many scientists, in particular in nanoscience and condensed matter physics, want to see their work have societal impact. The nanoscience centers could help such researchers find avenues for contributions to solving problems related to solving energy problems.

There should be a continuing effort within DOE and between the centers to understand the complementary role among the three nanoscience centers. We discussed the balance between state-of-the-art and user-facility modes. Three centers may help in this respect in that the optimization need not take place at each center but on a national scale.

Specific comments on the Molecular Foundry: The organization of each thrust area (a prominent lead scientist, some staff scientists, post docs, and students) looks like a lean and efficient self-contained research operation. It looks less suited to handle a large throughput of users. There seems to be a tension between the stated mission and the organization that needs to be resolved.

Specific comments on the CINT: A forceful point was made that integration is central. In keeping with this vision, I would advocate that the concept of integration should include a plan to facilitate the adoption of the nano-scale science in technological applications. The university-business parks that were popular some years ago would perhaps be a model to consider.

Specific comments on the CNMS: I am enthusiastic about the prospects for applications of neutron scattering in nano-scale-science. Neutrons have been used in nanoscience for decades. The contributions are widespread; for example, the general area of polymer science has been and continues to be strongly affected by information obtained from SANS, where nano-scale structure can be determined in situ and in solution. The CNMS should be encouraged to pursue this special aspect of the center. Two areas deserve special mention. Neutrons have specific needs in terms of the nature and quantity of material needed for successful experiments. In many cases, the recipe is available, and it is a question of scaling. This is cost-effective and an area where CNMS could have a big impact on the scientific productivity of the ORNL-SNS campus. The other area is in helping to shape the suite of instruments for the SNS so that they can serve nanoscience. The SNS is in a state of high susceptibility now and needs input on the focus and emphasis of instruments. One of the ways to be involved is through an instrument development team (IDT) or an instrument advisory team (IAT). The CNMS needs to get involved early to shape the facility and they should be encouraged to submit a proposal to DOE for an instrument at the SNS and also (as mentioned in their white paper) pursue funding for specialized sample environments.

Richmond called for public comment. Scott Cram (LANL) said that he had run a research resource for 15 years. It has five components that all National Institutes of Health (NIH) resources have:

- Core research and development
- Collaborations
- Service
- Training
- Dissemination

He encouraged the Committee to look at this format for research centers. The balance between collaboration and service becomes self-limiting. The focus drifts toward collaborative projects. The Committee's concern about users is appropriate, but the tension between the two modes does tend to become self-limiting.

There being no further comments, Richmond adjourned the meeting at 10:45 a.m.

Respectfully submitted by

Frederick M. O’Hara, Jr.
Recording Secretary
Jan. 15, 2002