Report
to
Basic Energy Sciences Advisory Committee

Committee of Visitors
for
Basic Energy Sciences Chemistry Programs

March 25, 2002

I. Introduction

The National Science Foundation has long utilized Committees of Visitors to evaluate their research programs, the program quality, and the effectiveness of program administration. While these reviews are a statutory requirement for NSF, the reports of these committees have turned out to be extremely valuable to NSF, providing feedback on procedures, and also providing a window to the community to understand NSF processes. The relative homogeneity of NSF research programs and the straightforward focus on fundamental research make these committees especially effective.

The Office of Science within the Department of Energy is charged with funding fundamental research in support of the mission of the Department of Energy. It does so in a combination of university-sponsored research, research at national laboratories and user facilities operated at national laboratories. The heterogeneity of these programs, coupled with the mission issues, has been a significant contributor to the absence of such Committees of Visitors in the past. While there are regular external reviews of the national laboratory programs and the user facility programs at the national laboratories, there have been no reviews quite analogous to the National Science Foundation Committee of Visitor reviews.

Against this backdrop, the Director of the Office of Science requested that the Basic Energy Sciences Advisory Committee (BESAC) convene a Committee of Visitors to evaluate the programs within Basic Energy Sciences (BES). This report is an evaluation of the chemical sciences programs in the Basic Energy Sciences program, and is the first such committee report. It is organized in a fashion to show the charge to the Committee of Visitors, the composition of the Committee of Visitors, the evaluation process, and, finally, the recommendations and conclusions of the committee.

II. The charge

The review process began with a letter from the Director of the Office of Science, Martha Krebs, to the Chair of BESAC requesting that BESAC "establish a Committee of Visitors (COV) 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."

In response to this charge, BESAC appointed W. Carl Lineberger as Chair of the first evaluation committee, and sent a charge letter to establish such a committee, based upon the

principles outlined above. Specifically, the charge letter to the Committee of Visitors requests that the committee evaluate the Chemical Science programs of Basic Energy Sciences that are contained within the Fundamental Interactions Team and the Molecular Processes and Geosciences Team, as indicated below.

Fundamental Interactions Team
- Atomic, Molecular and Optical Physics
- Chemical Physics
- Photochemical and Radiation Sciences

Molecular Processes and Geosciences Team
- Catalysis and Chemical Transformations
- Separations and Analysis
- Heavy Element Chemistry
- Chemical Energy and Chemical Engineering

For these programs, the COV is requested to evaluate both the DOE laboratory projects and the university projects, assessing the efficacy and quality of the processes used to

- Solicit, review, recommend and document proposal actions
- Monitor active projects and programs
- Comment on how the award process has affected
  - The breadth and quality of the portfolio elements
  - The national and international standing of the portfolio elements

Finally, the charge letter requests a recommendation as to how this review process might be improved in the future. The full charge letter appears in Appendix I.

III. The Committee Composition

The breadth of the charge to the COV and the number of programs to be scrutinized suggested that the size of the committee would be substantial. Eventually, approximately 20 people were chosen to serve on the Committee of Visitors. As the documentation of the balance and the expertise of these committee members is a crucial component in validating the credibility committee's conclusions, the characteristics of the COV membership will be described in some detail.

As noted earlier, there were seven major areas that the COV was requested to evaluate. A primary requirement was that the committee has significant expertise across all of these areas, and that this expertise should not rely upon one person alone. A second requirement was that a significant fraction of the committee receives no direct research support from the Department of Energy. In the case of this committee, approximately 25% of the members, including the

Committee Chair, receive no support from DOE. It was also important to have representation on the COV from individuals with experience in managing research programs, either at DOE or NSF. There was an attempt to balance between university principal investigators and national laboratory investigators. A final overlay also considered a number of other balance factors, including institution, geographic region, etc. In the end, the COV constituted an exceptional group of internationally recognized researchers, with broad research expertise in the areas being reviewed, as well as a deep familiarity with DOE programs.

A committee was thus established, and the first committee meeting was scheduled for September 18-20, 2001. The events of September 11, 2001 forced the cancellation of this meeting and necessitated some reshuffling of committee membership as a new meeting date was chosen. As it turned out, nearly 90% of the originally selected committee members were able to attend the rescheduled COV meeting, January 30-February 1, 2002.

W. Carl Lineberger of the University of Colorado chaired the Committee of Visitors. The other committee members were divided into four subgroups, representing areas of COV primary expertise that coincided with the programs to evaluate. These subgroups, listed below, are the ones that carried out the initial, expert-based evaluation of the DOE programs, in a process described in the following section.

Group 1: Atomic, Molecular and Optical & Chemical Physics
- Professor Theodore E. Madey, Rutgers University – Chair
- Professor C. Lewis Cocke, Kansas State University
- Professor Stephen R. Leone, NIST and University of Colorado
- Professor Marsha I. Lester, University of Pennsylvania
- Professor Ann E. Orel, University of California Davis

Group 2: Separations and Analysis & Heavy Element Chemistry
- Professor John I. Brauman, Stanford University – Chair
- Dr. Carol J. Burns, Los Alamos National Laboratory
- Dr. Charles H. Byers, Oak Ridge National Laboratory
- Professor Graham R. Cooks, Purdue University
- Professor Robert T. Paine, University of New Mexico

Group 3: Photochemical and Radiation Sciences & Electrochemistry
- Professor Peter C. Ford, University of California Santa Barbara – Chair
- Professor Mostafa A. El-Sayed, Georgia Institute of Technology
- Professor Richard M Osgood, Columbia University and Brookhaven National Laboratory
- Professor Nicholas Serpone, Concordia University
- ~~Professor Henry White~~, University of Utah, - unable to attend

Group 4: Catalysis and Chem Transformations & Chemical Engineering
- Professor John C. Hemminger, University of California Irvine – Chair
- Professor Dennis W. Bennett, University of Wisconsin Milwaukee

~~Professor Malcolm Chisholm~~, Indiana University- unable to attend
Professor Gary L. Haller, Yale University
Professor Lawrence T. Scott, Boston College

IV. The process

The entire COV evaluation process required two and one-half days at the Germantown facility. The period to be evaluated covered FY 1998, 1999 and 2000. The review began with a general overview of the BES programs to be reviewed and a discussion of the review process. It was noted that the BES mission relevance for all projects being reviewed was taken for granted and was not a part of the review criteria. The committee did not consider any proposals that had been rejected for lack of BES mission relevance. As noted earlier, the Committee of Visitors was divided into four groups, with each group providing primary review of BES programs in their area of special expertise.

The materials that were provided for each of the groups included the following:

- Program summary
- List of all active university projects
- Approximately 12 university program jackets
    - Several easy "fund" and easy "decline" cases
    - Most jackets were "at the decision margin"
- All National Laboratory jackets with actions taken during this period
    - New initiatives
        - Proposals, site visit reports, recommendations
    - Continuing projects
        - Site visit reports, reviews, staff recommendations, and laboratory responses
- Any other materials requested by that group

Each expert group first met with the appropriate program managers to obtain further program briefings, and then proceeded to evaluate the program jackets provided to them. The subject matter expertise of the committee members made it possible to evaluate not just the procedures, but also issues such as the quality of referees selected, the breadth of referees, and the quality of the referee reports. In addition, the committee could reach an independent evaluation of the scientific judgment exercised by the Program Officer in making funding decisions. This expert group prepared preliminary conclusions and drafted a tentative set of conclusions. The Chair of this committee then briefed a second group, known as the Generalist Readers. This latter group was composed solely of individuals from the other three groups.

They reviewed exactly the same materials as the expert committee, to provide a crosscut "reality check" as to quality standards, management procedures, and completeness of decision documentation, and to obtain a sense of relative program quality at the decision margin.

Finally, the expert and generalist groups met to compare their conclusions and to prepare an overall set of summary views. At the end of this process, the Committee of Visitors gathered as a whole to discuss the subgroup findings, to identify common issues, and to agree upon overall conclusions. The findings of this last meeting form the primary basis for this report.

V. Discussion and Recommendations

The Committee of Visitors was pleased to conclude that, in the programs reviewed, the research portfolios were of very high quality. The research programs were, in general, very well managed, and were carrying out important, relevant science for the Department of Energy. The Committee of Visitors especially commended Dr. Dehmer for taking the lead in establishing this oversight process to improve and open the programs of the BES. The support for the Committee of Visitors provided by the BES staff was excellent.

There were a number of other conclusions and recommendations that were equally applicable to all of the programs that were evaluated. These common recommendations and the appropriate discussion are presented first, followed by a discussion of program-specific issues. These overarching recommendations include the need for standardized program documentation, comments on the program evaluation mechanisms, conclusions on program quality, discussion of BES staffing, and other program support issues.

Documentation

A primary conclusion of the COV was that the process of documentation of decisions, processes, reviews, etc. would benefit enormously from standardization across all of BES. This standardization would dramatically enhance the openness of the award process, and, at the same time, make it much easier for temporary program officers to rapidly and effectively carry out their jobs. The COV notes that the development of standardized material and the necessity for careful documentation are in the process of change in BES, and we could see evidence for such change in the folders that we examined. We encourage this process and urge even more change in this direction. Recommendations for standard documentation are indicated briefly below.

- Develop common forms for referee reports, solicitations, and all other repetitive activities. Make the report form such as to force the reviewer to make a recommendation.
- Develop a time/document line page for the front of every project jacket. This enables the ready determination of what actions, responses and materials are present.
    - Include all major events in the project proposal, review, reporting, and evaluation processes. list
    - The format should make it readily apparent when a major event did or did not occur.
- Develop procedures to ensure that all of the important documentation is present.
- Both university and laboratory activities will benefit from standardization.

While all programs will benefit from this standardization, the somewhat different nature of awards to university investigators and those to National Laboratory teams require some comment. Thus, our comments and recommendations specific to university or National Laboratory programs are summarized in the following list:

- University program documentation
    - Grants are primarily to individual investigators and follow long-established procedures.
    - Project documentation is generally appropriate and complete.
    - As decisions are generally simple "fund" or "decline" ones, the actions taken by program officers are clear and documented.
- National Laboratory program documentation
    - Programs involving new initiatives are generally well documented.
    - Continuing program documentation is less complete
        - As decisions on continuing multi-investigator laboratory programs are rarely simple "fund" or "decline" ones, the careful documentation of program officer and laboratory actions is critical.
        - Laboratory responses to site visits and DOE recommendations are often verbal. A uniform procedure involving written responses is needed.
        - More recent continuation decisions are better documented.

Program evaluation

The DOE programs are evaluated by a variety of complementary mechanisms, including mail reviews, site visits by teams of scientists, site visits by program officers, and contractor meetings. In general, the COV found these various evaluation mechanisms to be effective and appropriately utilized. The COV, however, noted several areas where minor modifications and extensions of the current mechanisms might benefit the overall program and possibly increase the number of new investigators in DOE programs. Our recommendations are concerned with contractor meetings and workshops, mail reviews, and the necessity for an effective referee information system.

- Contractor meetings and workshops play a key role in program definition.
    - These meetings are extremely valuable for both program evaluation and mission issues.
    - BES should consider expanding regular contractor meetings to additional programs.
    - Program officers should expand invitations to include more unfunded and/or young scientists, to help bring new blood into programs. The number of such invitees should be large enough and varied enough that the program officers cannot be considered to be "preselecting" new grantees.
    - Such meetings may also provide a mechanism to expand interest in fields vital to DOE.Using mail reviews to supplement laboratory site visits may be valuable in some cases.
- The selection of the best possible referees and the realization of the broadest referee base would be enormously aided by the existence of an effective information management system.

Program quality

The COV was very favorably impressed with the high quality of the BES-supported programs. Our overall program quality conclusions are as follows:

- The top DOE research programs are world-class, outstanding in any environment.
- For some program areas that we reviewed, increasing the grant size of the most highly ranked programs, even at the expense of not supporting some programs at the decision margin, could produce better science for DOE.
    - The COV recognizes that this is a complex area, as other factors, such as programmatic relevance, play a greater role at the margin. Nonetheless, we recommend careful exploration of this option.
    - In that grant size has not kept up with inflation, this possibility should be at least considered in all of the programs.
- In a period of flat overall funding, new initiatives can be used to invigorate programs, especially when they can assist the core programs. Successful examples of this approach include the AMO and nanoscience initiatives. We encourage BES to continue a broad approach to process where possible.

Staffing and program support

The COV relied heavily on the excellent BES staff to provide the documentation and statistical summary information that was necessary to carry out our assignments. As a result, we encountered several areas involving staff and support that affect the subject of the COV. The COV had strong feelings about issues involving the information management system and program officer rotators. As the COV requested data, we found that the current Office of Science information management system was almost an impediment to the program managers.

Specifically, we feel that the current Office of Science information management system appears to have number of problems. The deficiencies that we perceive include the following:

- Fails to provide needed reviewer data as to reviewer qualifications, selection, frequency of reviewer usage, reviewer responsiveness, quality of reviewer judgments.
- Fails to provide useful guidance to new rotators in reviewer selection.
- Fails to provide current or historical program support data in searchable, analyzable forms.
- Forces program officers to develop parallel information management systems.
- Makes it very difficult for program rotators to take advantage of prior experience, contributing to referee selection issues.

The shortcomings of this system have a pervasive effect, as the staff is already overworked, and the lack of needed information adds to the problem. The COV also notes an urgent need to fill current BES staff vacancies. In a broader context, there are critical needs to find ways to recruit new rotators, and to find mechanisms to allow them to function effectively and rapidly in their new environment.

Finally, the COV notes that the NSF Fast Lane electronic information system provides for electronic capture of much of the data that the COV requested and that the DOE staff could use effectively in carrying out its duties. This system also provides an important outside transparency to agency actions. While it may not be feasible (or desirable!) to port Fast Lane from NSF to the DOE Office of Science, the dedication of significant DOE staff effort to increasing Web-based proposal and review activities could be very beneficial for both DOE staff and grantees.

The COV Process Itself

The Committee of Visitors viewed this process as informative to them and, hopefully, useful to the Office of Basic Energy Sciences. It is our strong recommendation that this process should be continued in the future, especially if BES can utilize the views and recommendations of the Committee of Visitors. The COV notes that this process provides a (what is grpa?) GPRA-like overview of the BES programs and, at the same time, helps to remove any mystery associated with the grant award process. Over time, the exposure of many members of the community to this review process will greatly improve the information flow.

Future COVs will definitely benefit from this first round of program review. They should receive materials that are better focused on well-defined tasks. They would receive the prior COV report and be afforded the opportunity to review the various responses to the report. Overall, the COV process will certainly work to enhance both the efficiency and the openness of BES programs. The COV is convinced that establishing a regular external review process such as this one would benefit most other research activities within the Department of Energy.

Program-specific recommendations

In addition to these overall conclusions and recommendations, the COV reached a number of conclusions that were specific to individual programs, and made a number of observations and recommendations that were program-specific. This material is presented in the following set of bulleted lists. Hopefully, the absence of a fuller discussion of each program should not detract from the recommendations.

AMO Physics and Chemical Physics

- These are very strong, active, well managed programs.
- The science being supported is uniformly viewed as first rate.
- There are significant numbers of new investigators and projects.
- A DOE-sponsored AMO Workshop in 1997, together with a new AMO initiative, has produced dramatic changes in this program, and serves as a model for revitalization.

Chemical Engineering

- This is a small program, with some strong projects.
- The research activities are quite narrowly focussed, compared with the program name.
- Both new starts and turnover have been extremely low for a number of years.
- It may be advantageous to incorporate this activity into larger BES programs.

Photochemistry and Radiation Science

- This is a very strong, well-managed program, carrying out first-rate science.
- The COV generally found very high quality, thoughtful proposal reviews.
- The regular contractor meetings for each program are very effective.

Separations and Analysis

- The most highly ranked programs are outstanding.
- The program is well managed.
- It seems possible that better science would result from increasing some of the best programs, using funds from programs at the margin.

Electrochemistry

- This is a fairly small program.
- Electrochemistry is a very important basic and applied program area for BES.
- The current mix of projects needs strengthening on fundamental aspects of field.
- Holding broadly based regular workshops with outside participation could expand program vision, as occurred with AMO.
- The documentation of funding decisions needs to more clearly address basis for actions taken, especially when diverse views are found in the reviews.

Heavy Element Chemistry

- This is a relatively small program, but DOE is the national supporter of the entire field.
- This subject is very important for DOE programs.
- There are small numbers of investigators in field, with consequent low proposal pressure from universities.
- The program would benefit from regular workshops, both for program definition and to encourage new persons into the field.

Catalysis and Chemical Transformations

- The program is supporting a very good balance of programs.
- The program appears strong and healthy, with reasonable turnover.
- The program is well managed.

VI. Conclusion

The Committee of Visitors for Chemistry programs has appreciated the opportunity to work with the BES leadership in this first external review of their procedures. We have learned an enormous amount, and we hope that BES can utilize our suggestions. This open evaluation of programs can only improve both the programs and the external appreciation of them. We believe that all mission-driven science programs would benefit tremendously from such open evaluation.

Appendix I. COV Charge Letter

UNIVERSITY OF OREGON

24 April 2001

W. Carl Lineberger
Department of Chemistry and JILA
JILA, CB 440
University of Colorado
Boulder, CO 80309-0440

Dear Dr. Lineberger:

The Basic Energy Sciences Advisory Committee (BESAC) has been charged by the Office of Science to assemble a Committee of Visitors (COV) to review the management processes for components of the Chemical Sciences, Geosciences, and Biosciences Division of the Basic Energy Sciences (BES) program. Thank you for agreeing to chair this BESAC COV panel. Through your leadership, the panel should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. I would like the panel to consider and provide evaluation of the following four major elements.

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
   (a) solicit, review, recommend, and document proposal actions and (b) monitor active project and programs.

2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
   (a) the breadth and depth of portfolio elements, and
   (b) the national and international standing of the portfolio elements.

3. Comment on future directions proposed by the Division and BES management and on opportunities that might not have been presented.

4. Comment on how the process for these reviews might be improved.

The panel should assess the operations of the programs during the fiscal years 1999 and 2000. The panel may examine any files during this period for both DOE laboratory projects and university projects. The components of the Division that you are being asked to review are:
(1) Atomic, Molecular, and Optical Sciences
(2) Chemical Physics
(3) Photochemical and Radiation Sciences

DEPARTMENT OF CHEMISTRY
College of Arts and Sciences · 1253 University of Oregon · Eugene OR 97403-1253 TELEPHONE - (541) 346-4601
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(4) Catalysis and Chemical Transformations
(5) Separations and Analysis
(6) Heavy Element Chemistry
(7) Chemical Engineering and Chemical Energy.

You will be provided with background material on these program elements prior to the meeting.

The COV is scheduled to take place September 19-21 at the BES/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A presentation to BESAC is requested at the February 2002 meeting. Following acceptance of the full BESAC committee, the COV report with findings and recommendations will be presented to the Director of the Office of Science.

If you have any questions regarding BESAC, its legalities or logistics, please contact Sharon Long, Office of Basic Energy Sciences at 301-903-5565 or by e-mail at sharon.long@science.doe.gov. With questions related to the Division of Chemical Sciences, Geosciences, and Biosciences, please contact William Millman , 301-903-5805, william.millman@science.doe.gov.

Sincerely,

Geraldine Richmond

Geraldine Richmond, Chair
Basic Energy Sciences Advisory Committee

cc:
P. Dehmer
I. Thomas
S. Long

Appendix II. COV Membership

W. Carl Lineberger, University of Colorado, Chair

Professor Dennis W. Bennett, University of Wisconsin Milwaukee
Professor John I. Brauman, Stanford University
Dr. Carol J. Burns, Los Alamos National Laboratory
Dr. Charles H. Byers, Oak Ridge National Laboratory
~~Professor Malcolm Chisholm~~, Indiana University- unable to attend
Professor C. Lewis Cocke, Kansas State University
Professor Graham R. Cooks, Purdue University
Professor Mostafa A. El-Sayed, Georgia Institute of Technology
Professor Peter C. Ford, University of California Santa Barbara
Professor Gary L. Haller, Yale University
Professor John C. Hemminger, University of California Irvine
Professor Stephen R. Leone, NIST and University of Colorado
Professor Marsha I. Lester, University of Pennsylvania
Professor Theodore E. Madey, Rutgers University
Professor Ann E. Orel, University of California Davis
Professor Richard M Osgood, Columbia University and Brookhaven National Laboratory
Professor Robert T. Paine, University of New Mexico
Professor Nicholas Serpone, Concordia University
Professor Lawrence T. Scott, Boston College
~~Professor Henry White~~, University of Utah, - unable to attend

Appendix III. **COV Meeting Agenda**

Basic Energy Sciences Advisory Committee -- Committee of Visitors
January 30- February 1, 2002

January 29

7:30 – 9PM	Informal Gathering at Marriott	COV/BES Leadership

January 30

8:15	Welcome and Introduction	Pat Dehmer
8:45	A Historical Perspective	Bill Kirchhoff
9:10	Chemical Science Overview	Bill Millman
9:30	Fundamental Science	Al Laufer
10:00	Molecular Processes and Geophysics	Bill Millman
10:30	Breakout Session I Chair discussion of procedures 20 minute staff presentation on program, important issues, Divide up programs so that each jacket has 2 readers Read till lunch	Primary Groups appropriate staff
12:30	Lunch	
1:30	Breakout Session I (continued) Complete reads; discuss each jacket as a group, led by readers Outline big picture of program Assign drafting responsibilities of each area on templates	
3:45	COV Executive Session	
4:15 – 4:45	COV meets with BES staff raises any issues that need addressing determine what additional materials, information are required	
4:45	Transport to Hotel	
6:00 – 9:00	Dinner with BES staff	

January 31

8:30 – 11:30	Draft first read report	Primary Groups
11:30	First Read Chair gives overview to Second Read Panel	Second Groups
12:00	Lunch	
1:00	Begin Second Read 20 min review of program and issues by staff limited mission of second read groups: **1.** assess work of 1st read group **2.** Compare program quality across boundaries This will go in a separate section on template	Second Groups
4:00	Second Read Drafts Section	Second Groups
5:00	Transport to Hotel	
6:00– 9:30	Working dinner brief reports by each Chair group discussion of common issues/findings opportunity for Chairs to get any final assignments/issues in order	COV only

February 1

8:30	Prepare Merged Reports Writing period Consult with second read chairs DOE staff available for information	
10:30	COV Executive Session discuss final conclusions and recommendations prepare for discussion with BES leadership what COV procedures would be better in the future?	COV
11:30	Verbal Report to BES Leadership present snapshot of conclusions, recommendations an opportunity to learn if issues need elaboration, clarification	
12:00	Adjourn	

COV Assignments to Panels

Atomic, Molecular and Optical & Chemical Physics

Expert Readers	Generalist Readers
Ted Madey (Chair)	Mostafa El-Sayed (Chair)
Lew Cocke	Carol Burns
Steve Leone	Graham Cooks
Marsha Lester	John Hemminger
Ann Orel	Larry Scott

Separations and Analysis & Heavy Element Chemistry

Expert Readers	Generalist Readers
John Brauman (Chair)	Steve Leone (Chair)
Charles Byers	Dennis Bennett
Carol Burns	Peter Ford
Graham Cooks	Nick Serpone
Robert Paine	

Photochemical and Radiation Sciences & Electrochemistry

Expert Readers	Generalist Readers
Peter Ford (Chair)	Gary Haller (Chair)
Mostafa El-Sayed	John Brauman
Rick Osgood	Charles Byers
Nick Serpone	Lew Cocke
	Marsha Lester

Catalysis and Chemical Transformations & Chemical Engineering

Expert Readers	Generalist Readers
John Hemminger (Chair)	Rick Osgood (Chair)
Dennis Bennett	Robert Paine
Gary Haller	Ted Madey
Larry Scott	Ann Orel

August 10, 1999

Professor Geraldine L. Richmond
Chair, Department of Chemistry
University of Oregon
Eugene, OR 97403-1253

Dear Geri:

I very much appreciate your willingness to serve a second term as Chair of the Basic Energy Sciences Advisory Committee (BESAC). I believe that the continuity in leadership that you will provide will be critical during the coming year as BESAC completes its study of the electron beam microcharacterization centers and begins its new activities. Under your leadership during the past year, BESAC activities have produced extraordinary results that already have -- and will continue to have -- broad impacts in the Basic Energy Sciences program. I especially want to acknowledge BESAC's help in the review of the programs and operations of the High Flux Isotope Reactor at Oak Ridge National Laboratory; the determination of the appropriate five-year R&D agenda for novel, coherent light sources ("4th generation" light sources); and the identification of the forefront of the physical and biophysical sciences in the area of complex systems through BESAC's help with the organization of and the participation in the workshop at Lawrence Berkeley National Laboratory.

During the coming year, I would like BESAC to advise me on the current status of the Advanced Light Source and to take on a new and continuing charge to oversee Committees of Visitors for the Basic Energy Sciences (BES) Program. I have provided an overview of each activity below. You should develop the detailed charges through discussions with the chair of the panel, committee, or workshop and the Associate Director of BES.

The first activity is a review of the Advanced Light Source to examine those issues that were raised by the BESAC Report on "DOE Synchrotron Radiation Sources and Science," known as the Birgeneau Report. In particular, BESAC should explore ALS's vision for the future, the quality and diversity of science programs at the facility, the user demand, and the interactions and relationship with the user community.

The second activity is the establishment of Committees of Visitors (COVs) through which BESAC can provide an assessment on a regular basis of matters pertaining to program decisions. COVs should review program management every three to four years on a rotating basis for major elements of the BES program selected by the Associate Director for BES. The COVs should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs. You should work with the Associate Director for BES to establish the processes and procedures for the first COV to occur in 2000.

I appreciate BESAC's willingness to take on these important activities, and I look forward to meeting with you and learning of your progress throughout the coming year.

Sincerely,

Martha A. Krebs
Director
Office of Science

COV Report to BESAC

W. Carl Lineberger

February 25, 2002

COV for DOE Chemistry Programs

- The history
- The charge
- The committee
- The process
- The recommendations
  - General
  - Program specific

History of COV at DOE

- This is the first external evaluation

The COV Charge (I)

- *From Director of the Office of Science to Chair, BESAC:*
- Establish a “committees of visitors (COV) 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.”

The COV Charge (II)

- *From Chair, BESAC to Chair, COV:*
- For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
  - Solicit, review, recommend and document proposal actions and
  - Monitor active projects and programs
- Within the boundaries defined by DOE missions and available funding, 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 Charge (II)

- Comment on future directions proposed by the division and BES management and on opportunities that might not have been presented.
- Comment on how the process for these reviews might be improved

Programs to Review

- **Fundamental Interactions**
  - **Atomic, Molecular and Optical Physics** — Group 1
  - **Chemical Physics** — Group 1
  - **Photochemical and Radiation Sciences** — Group 2
- **Molecular Processes and Geosciences**
  - **Catalysis and Chemical Transformations** — Group 4
  - **Separations and Analysis** — Group 3
  - **Heavy Element Chemistry** — Group 3
  - **Chemical Energy and Chemical Engineering** — Group 4

The COV Itself

- Twenty experienced, well respected individuals
- About 25 % receive no DOE support
- Attempt balance among many factors
  - Research area
  - University investigators
  - National Laboratory investigators
  - Prior DOE/NSF program management experience
- Divided into four disciplinary groups
- Scheduled September 18th meeting cancelled, with resulting replacement of a few members

Group 1: Atomic, Molecular and Optical & Chemical Physics

- Ted Madey – Chair
- Lew Cocke
- Steve Leone
- Marsha Lester
- Ann Orel

Group 2: Separations and Analysis & Heavy Element Chemistry

- John Brauman – Chair
- Carol Burns
- Charles Byers
- Graham Cooks
- Robert Paine

Group 3: Photochemical and Radiation Sciences & Electrochemistry

- Peter Ford – Chair
- Mostafa El-Sayed
- Rick Osgood
- Nick Serpone
- ~~Henry White~~

Group 4: Catalysis and Chem Transformations & Chemical Engineering

- John Hemminger – Chair
- Dennis Bennett
- ~~Malcolm Chisolm~~
- Gary Haller
- Larry Scott

The 2 ½ Day COV Process

- General BES presentation to full COV
- Separate into “expert” breakout groups, e.g., 1
  - Meet with appropriate program managers
  - Evaluate jackets by requested criteria
  - Draft report – chair briefs second read group
- Second read – members from other groups (e.g., 2,3,4)
  - Review same materials to provide crosscut “reality check”
    - Research quality standards
    - Procedural standards
- Merge to produce a final group report
- Meet as a whole to identify common issues

Materials Provided for Each Group

- BES mission relevance for all projects predetermined
- FY 1998, 1999, 2000
- Approximately 12 University program jackets
  - Listing of **all** active projects
  - Several easy fund and easy “decline” cases
  - Most jackets were “at the decision margin”
- All National Laboratory jackets
  - New Initiatives
    - Proposals, site visits, recommendations
  - Continuing projects
    - Site visit reports, reviews, staff recommendations, lab responses

The COV Recommendations

- General observations
- General recommendations
- Program specific recommendations

- This is a preliminary report, to obtain feedback from BESAC on areas to emphasize, clarify . . .

General Observations

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

Classes of General Recommendations

- Standardized program documentation
- Program evaluation mechanisms
- Program quality conclusions
- BES staffing and program support issues
- The COV process itself

Standardized Documentation (I)

- Develop common forms for referee reports, solicitations, and all other repetitive activities. Make the report form such as to force a recommendation.
- Develop a time/document line page for the front of every project jacket. This enables the ready determination of what actions, responses and materials are present.
  - Include all important events in project.
  - Make apparent when something did or did not take place.

Standardized Documentation (II)

- University program documentation
  - Following long-established procedures
  - Project documentation generally appropriate and complete
- National Laboratory program documentation
  - New initiatives generally well-documented
  - Continuing program documentation less complete
    - Laboratory responses to site visits /DOE Recommendations are often verbal, rather than written
    - Accomplishment-based emphasis for laboratory programs
    - More recent continuation decisions are better documented
- Both university and laboratory activities will benefit from standardization

Program evaluation mechanisms

- Contractor meetings and workshops
  - Extremely valuable for evaluation and mission issues
  - Consider expanding to more programs
  - Invite some unfunded and/or young scientists to help bring new blood into programs
- Mail reviews to supplement laboratory site visits will be useful in some cases
- An effective information management system could be invaluable to staff in assisting the selection of the best program reviewers

Program quality conclusions

- Top DOE research programs are world-class, competitive and outstanding in any environment
- For some areas, increasing grant size at the expense of programs at the decision margin might well produce better science for DOE
  - This is a complex area, as programmatic relevance is not a simple binary choice, as COV has assumed.
- New initiatives can invigorate programs, especially when they can assist the core programs
  - AMO, nanoscience . . .

Staffing and Program Support Issues

- Current Office of Science information management system
  - Fails to provide needed reviewer data
    - Selection, frequency of usage, responsiveness, quality of judgments
  - Fails to provide current or historical program support data in searchable, analyzable forms
  - Forces program officers to develop parallel systems
  - Makes it very difficult for program rotators to take advantage of prior experience, contributing to referee selection issues
- Staff is already very overworked, and adding new reporting responsibilities is not obviously helpful
- Urgent need to fill BES staff vacancies
- Urgent need to find ways to recruit new rotators, and to find mechanisms to allow them to function effectively and rapidly in their new environment

The COV Process Itself

- Viewed as informative and useful
  - Should be continued, if DOE can utilize the COV views
  - Provides a GPRA-like overview of programs
- Next COV will benefit from this first round
  - Receive materials better focussed on task
  - Receive prior COV report and BES responses
- COV would likely benefit most other areas in DOE

Program-specific Recommendations

- AMO Physics and Chemical Physics
  - Very strong, active, well managed programs
  - Science viewed as first rate
  - Significant numbers of new investigators and programs
  - DOE-sponsored AMO Workshop in 1997, together with new initiative, has produced dramatic improvement
- Chemical Engineering
  - Small program, with some strong projects
  - Activities are narrow compared with program name
  - Both new starts and turnover are extremely low
  - Perhaps better to incorporate into larger BES programs

Program-specific Recommendations

- Photochemistry and Radiation Science
  - Very strong, well-managed program with first-rate science
  - Very high quality, thoughtful proposal reviews
  - Very successful annual contractor meetings
- Separations and Analysis
  - Top programs are outstanding
  - Well managed
  - Possibly better science would result from increasing some of the best programs using funds from programs at the margin

Program-specific Recommendations

- Electrochemistry
  - Fairly small program
  - Very important basic/applied program area for BES
  - Needs strengthening on fundamental aspects of field
  - Broadly based regular workshops with outside participation could expand program vision, as occurred with AMO
  - Funding decision documentation needs to more clearly address basis for actions taken

Program-specific Recommendations

- Heavy Element Chemistry
  - Relatively small program
  - Very important for DOE programs
  - Small numbers of investigators in field
  - Would benefit from regular workshops
- Catalysis and Chemical Transformations
  - Very good balance of programs
  - Strong and healthy
  - Well-managed

In Conclusion

- The Committee of Visitors for Chemistry programs has appreciated this opportunity to work with BES leadership in this first external review of their procedures. We have learned an enormous amount, and believe that all mission-driven science programs would benefit tremendously from such open evaluation.

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