



**Report of the Committee of Visitors of the
Division of Chemical Sciences, Geosciences, and
Biosciences**

to the

Basic Energy Sciences Advisory Committee

Review of FY 2005, 2006, and 2007

April 23-25, 2008

Germantown, MD

Executive Summary

A Committee of Visitors (COV) participated in a review of the programs in the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the Office of Basic Energy Sciences (BES) over the years of 2005, 2006 and 2007. Thirty-four participants were involved in this review that took place in Germantown on April 23-25, 2008. The charge given to the COV from John Hemminger, the COV Chair of the Basic Energy Sciences Advisory Committee (BESAC), was to assess (1) the efficacy and quality of the processes used to solicit, review, and reach decisions on proposals, document decisions, and monitor progress on funded proposals; (2) how the award process has affected the breadth and depth of portfolio elements, including the national and international standing of these elements within the boundaries of DOE missions and available funding; and (3) the programs' progress in achieving those BES long-term goals that are tracked by the Office of Management and Budget. The format was similar to previous COV reviews of programs in the Office of Science.

Overall, the COV was very impressed with the management and decision making processes reviewed in the CSGB Division. The proposal solicitation, review, and award process was found to be managed very well, primarily as a result of the high caliber of both the division management and the program managers. The CSGB Division is funding individuals and programs that have high levels of national and international standing. The seven programs were individually rated with respect to the four long-term goals of the Office of Basic Energy Sciences. The rating was "Excellent" in 23 out of the 24 entries! This remarkable set of excellent ratings should be viewed with much pride by BES and the Office of Science as the COV members believe that this is a true representation of the Division's progress towards its long-term goals. The COV was also very appreciative of the high degree of organization of Division management and staff during the review and their responsiveness to all requests.

The COV makes only one recommendation. The members chose to limit themselves to a single recommendation in order to emphasize the overarching importance that they believe this issue has to the CSGB Division and the impact it has on their ability to manage effectively its programs. The COV recommends, *in the strongest terms*, the rigorous collection of data on all aspects of proposal solicitation, review, funding recommendation, proposed action and all metrics associated with progress that can assist in the evaluation of the impact of funded work. Collection of such information requires the development and implementation of an electronic data management system that can be coordinated with other information-collecting activities in BES and the Office of Science. Such information should include new investigators to DOE and the program, publications, patents, presentations, awards, commercialization successes, new collaborations, annual reports/abstracts from contractors meetings, personnel on project, technical highlights, information on PI (institution, demographics), number of years funded, and funding profile. Information systems should also be used to collect a distinct set of information on reviewers: institution, BES funded/non-funded, frequency of use, demographics, etc. The implementation of such an information management system will bring many benefits to the management and program managers of the Division including improving the consistency of documenting of proposal decisions and providing a dependable resource for selecting reviewers and facilitating the compilation and communication of the accomplishments of funded programs. If implemented throughout the Office of Science it will enable a rapid response (with updated documentation) to changing national priorities and will provide data that maps the progress of

Office of Science programs towards high-level goals. Such a data system would also provide links across DOE documenting the impact of DOE science and its relationship to other programs, which is particularly important for communicating with the public and Congress.

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I. Introduction, COV Membership and the COV Review Process

A Committee of Visitors (COV) participated in a review of the programs in the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the Office of Basic Energy Sciences program over the years of 2005, 2006 and 2007. Thirty-four participants were involved in this review that took place in Germantown on April 23-25, 2008. The charge of the COV was to assess (1) the efficacy and quality of the processes used to solicit, review, and reach decisions on proposals, document decisions, and monitor progress on funded proposals; (2) how the award process has affected the breadth and depth of portfolio elements, including the national and international standing of these elements within the boundaries of DOE missions and available funding; and (3) the programs' progress in achieving BES long-term goals that are tracked by the Office of Management and Budget. The COV members (Appendix A) were selected for their scientific expertise by COV Chair Geri Richmond in consultation with CSGB personnel. Additional considerations were given to achieving a balance in terms of (1) those receiving BES support *vs.* those not receiving support; (2) members from universities, national labs and federal institutions, and industry; and (3) gender and race diversity. Each COV member was assigned to one of six subpanels representing the nine programs. A chair was selected for each subpanel that was responsible for producing a written summary of findings, comments, recommendations, and ratings of progress toward achieving long-range BES goals. The agenda of the meeting is in Appendix B.

The evaluation of the programs followed the process established by the 2005 CSGB Division COV. The most extensive examination of the programs occurred in the "First Read" of the portfolio of activities in those programs most closely related to the expertise of the participating COV panelists. Panel members as a group of 5-6 completed the COV Template (Appendix C) with their findings, recommendations and comments. When this read was completed, the panels shared their results with the entire COV. This was followed by a "Second Read" by a largely different group of panelists with less expertise in the programs that they were evaluating. Their findings, recommendations and comments were merged with the documents produced in the First Read. The individuals on each of the panels are listed in Appendix A. The completed templates containing the evaluative comments of the combined panelists for each of the 6 groups are given in Appendix D. Panelists were also asked to rate the progress of each program toward BES's long-term goals. The results are summarized in Appendix E.

II. Major Findings, Comments, and Recommendations of the COV

A. Major Findings of the COV

1. We find that across the CSGB Division the quality of the decision making processes and documentation made by the program managers is outstanding, reflecting their experience and professionalism. This performance is particularly noteworthy given the lack of an effective electronic information system, and the uncertainties in the budget.
2. Overall, our impressions of solicitation, review, recommendation, and documentation of

portfolios were very favorable. We were generally impressed in many cases with the quality and number of reviewers used in many programs, the depth of analysis by the program managers, the documentation and the overall funding decision.

3. Monitoring of active projects and programs is occurring, but the documentation of this activity suffers seriously from the lack of a comprehensive database that collects from the PIs such information as publications, presentations at meetings, awards, funded students and personnel funded, and progress towards other metrics. There has been an increase in the use of contractors meetings as a mechanism for monitoring the progress of PIs which we applaud and enthusiastically support. Such meetings have the added benefit of cross fertilization of ideas, particularly when individuals outside of the funded program are included.
4. Although understanding the review process is relatively straightforward for individual PIs, the COV found more ambiguities about the criteria used by reviewers in evaluation of national laboratory programs. For example, on-site reviews are an important part of the evaluation of ongoing programs at the laboratories, but are more likely to overemphasize past accomplishments. We encourage the CSGB program to direct members of on-site review panels to strive for a better balance between “forward looking” proposed science and track record in their evaluations.
5. We find overall that the science supported by the nine programs in the CSGB division consistently reflects both a high degree of intellectual depth and scientific breadth. The portfolios include scientists who are highly regarded on both the national and international level. However, our “findings” of the evolution of the portfolio with respect to new investigators, and to the diversity of investigators, are almost reduced to an anecdotal level due to the lack of an electronic information system that can readily gather this information on a comprehensive and historical level.
6. We find that, with the exception of the development of an electronic database system, we find that significant progress has been made since the last COV in a number of areas, including improvement in proposal solicitation, a re-evaluation and refocus of the Energy Biosciences program, timely filling of vacant program manager positions, including three new program manager positions, and program prioritization. We are encouraged by the addition of new staff positions in the Division and see this as an essential component of the new structure and priorities of the division. We are nevertheless surprised by the lack of any staff person in information technology in the division and encourage immediate hiring of staff in this area.
7. We find that the several failures to fund major new initiatives after proposal solicitation and review have had a serious negative impact on the ability to bring many new investigators into the system and to potentially increase the diversity in terms of age, racial, and gender diversity of the portfolio.

B. Recommendation of the COV

The COV recommends, in the strongest terms, the rigorous collection of data on all aspects of proposal solicitation, review, funding recommendation, proposed action, and all metrics associated with progress that can assist in the evaluation of the impact of funded work. Such information should include new investigators to DOE/program, publications, patents, presentations, awards, commercialization successes, new collaborations, annual reports/abstracts from contractors meeting, personnel on project, technical highlights (“nuggets”), information on PI (institution, demographics) number of years funded, and funding profile. Information systems should also be used to collect a distinct set of information on reviewers: institution, BES funded/non-funded, frequency of use, demographics, etc. **Given the consistent recommendations of previous COV reports on this topic, it is time that the Office of Science rectifies this inadequacy. We cannot emphasize too strongly our expectation that by the time of the next COV review in three years significant progress will finally have been made toward meeting the repeated recommendation on this topic (see below) of the many COVs that have gone before us in the Office of Science.**

Using this database, COV strongly encourages the collection of the demographics associated with projects funded by the programs in a manner that is consistent with federal law. We also strongly encourage the programs to continue to enhance the representation of women and underrepresented minorities in their portfolios, and encourage these programs to continue to increase the number of new young investigators in their portfolios.

The implementation of such an information management system will bring many benefits to the management of the Division, and could address minor concerns that arose during the deliberations of some panels associated with this Committee. These benefits include improving the consistency of documenting proposal decisions, providing a dependable resource for selecting reviewers for all Division staff, and facilitating compilation and communication of the considerable accomplishments of the funded investigators in these programs.

For the record, Recommendations from previous COVs on this issue include:

From the 2005 COV Report of the CSGB of BES:

“COV strongly recommends the development of standardized database software and a coherent BES-wide computer database that would include information on reviewers, proposal tracking, documentation of decisions, and funding history and productivity of investigators. The establishment of an effective database is seen by the COV as mandatory to the effective management of a program as diverse and complex as the BES research portfolio.”

From the 2003 COV Report of the Department of Material Science and Engineering of BES:

“The Office of Science information management system is **ineffective** in many ways. ...Such a database is essential for the program managers to perform their jobs. The result of the present ineffective database (IMSC) is that many program managers have developed their own “shadow” systems. Such “shadow” systems take valuable time and effort to develop and are

of uneven quality and usefulness. In addition to increasing the effectiveness of a program manager, a high quality database on all the BES research programs would greatly enhance the development of reporting statistics that would be invaluable for a review such as this COV.”

From the 2002 COV Report of the CSGB of BES:

“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.”

From the 2007 COV Report of the Climate Change Research Division of Basic Energy Research (BER)

“This COV is making recommendations that require additional staff and support, including the development of more complete project dossiers and the development or acquisition of electronic document management and database systems for tracking, recordkeeping and oversight.”

From the 2005 COV Report of the Life Sciences Division of BER

“The COV is aware that a prior COV has recommended that BER set goals for, and keep records of, funding demographics in terms of underrepresented groups, junior scientists, and new investigators/independent viewpoints. The COV is also aware that BER has indicated that this is not permitted under current DOE operating guidelines. Without wishing to unduly flog a dead horse, this COV suggests that, given the strong initiatives elsewhere in the government in support of ensuring diversity in the Nation’s research community, that BER should perhaps seek a reconsideration of this issue by DOE leadership.”

From the 2004 COV of the Environmental Remediation Sciences Division of BER: “The COV believes it would be very useful if the research programs supported by BER were to set goals for, and keep records of, funding demographics in terms of underrepresented groups, junior scientists, and new investigators/independent viewpoints. If at all possible, all of SC should follow the example of the National Science Foundation and collect such information at the time each application is submitted in a way that can be included in a statistical database without being included in the tracking folder.”

From the 2007 COV of the Office of High Energy Physics Committee of Visitors Report

“We recommend that documentation and access to program data continues to be improved and that data is put into electronic form where this is not yet the case (the university grants program being one example).”

From the 2007 COV Report of the Office of Nuclear Physics

“We recommend a more extensive database of the information contained in the university grants, to facilitate tracking of the overall health of the program. Statistical data such as the number of PI’s per grant, average grant size, and time to notification of a proposal action are among the statistics that would be valuable to track.”

From the 2007 COV Report of the Office of Nuclear Physics

“There were several instances where the COV felt that **statistics would have been helpful in the evaluation process, as well as to DOE programs managers.** For example, the fraction of projects that are renewed, funding awarded versus funding requested, the correlation between ratings and funding, the duration of contracts that do not undergo competitive review, and demographics for awards. This should not be considered an exhaustive list, but rather examples of statistics that would be useful.”

III. Ratings of Progress Toward Long-Term Goals of OBES by Program

The COV was asked to rate each of the programs reviewed with respect to their progress in meeting the long-term (by 2015) goals of the Office of Basic Energy Sciences. The four goals are as follows:

***Goal a.** By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy related applications.*

***Goal b.** By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self assembling, and biological systems.*

***Goal c.** By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.*

***Goal d.** By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.*

The ratings [Excellent, Effective, Insufficient, Not Applicable (N.A.)] are listed in the table below. Detailed justifications for each rating are given in Appendix E.

Ratings given by the 2008 COV

Program Areas	Goal a	Goal b	Goal c	Goal d
<i>AMO Science/Gas-Phase Chemical Physics</i>	Excellent	Excellent	Excellent	Excellent
<i>Photochemistry/Condensed Phase Chemical Physics</i>	Excellent	Excellent	Excellent	Excellent
<i>Catalysis</i>	Excellent	Excellent	Excellent	Excellent
<i>Heavy Element Chemistry/Separations and Analysis</i>	Excellent	Excellent	Excellent	Excellent
<i>Geosciences</i>	Excellent	Excellent	Excellent	Excellent
<i>Biosciences</i>	Excellent	Excellent	Good	Excellent

Appendix A:

FY2008 Committee of Visitors for SC-22.1 Panel Membership, March 2008 Chemical Sciences, Geosciences, and Biosciences Division

Geri Richmond COV Chair Univ of Oregon
<http://richmondscience.uoregon.edu/>

AMO Sciences/Gas Phase Chemical Physics

Carl Lineberger Panel Lead University of Colorado
<http://jilawww.colorado.edu/wclgroup>

Tom Gallagher Panelist University of Virginia
<http://www.phys.virginia.edu/People/personal.asp?uID=tfq>

Anthony Johnson Panelist University of Maryland
<http://www.umbc.edu/caspr/johnson%20bio.html>

Arthur Suits Panelist Wayne State University
http://suitsmac.chem.wayne.edu/~r4/asweb/public_html/

Sotiris Xantheas Panelist Pacific Northwest Nat Lab
http://www.pnl.gov/science/staff/staff_info.asp?staff_num=5610

Photochemistry/Condensed Phase Chemical Physics

Peter Rossky Panel Lead University of Texas
http://www.cm.utexas.edu/directory/peter_rossky

Luis Echegoyen Panelist NSF/Clemson University
http://chemistry.clemson.edu/people/luis_echegoyen.htm

Etsuko Fujita Panelist Brookhaven Nat Lab
<http://www.bnl.gov/chemistry/bio/FujitaEtsuko.asp>

Devens Gust Panelist Arizona State University
<http://photoscience.la.asu.edu/photosyn/faculty/gust/indexR.htm>

Sharon Hammes-Schiffer Panelist Penn State
<http://research.chem.psu.edu/shsgroup/index.html>

Thom Orlando Panelist Georgia Tech
<http://www.chemistry.gatech.edu/faculty/Orlando>

Catalysis

Bruce Gates Panel Lead University of California, Davis
<http://www.chms.ucdavis.edu/research/web/catalysis>

Cynthia Friend Panelist Harvard University
<http://www.chem.harvard.edu/groups/friend>

Horia Metiu Panelist University of Cal., Santa Barbara
<http://www.chem.ucsb.edu/people/faculty/metiu/index.shtml>

Umit Ozkan Panelist Ohio State University
<http://www.chbmeng.ohio-state.edu/people/ozkan.html>

Simon Bare	Panelist	UOP, LLC
	Simon.Bare@uop.com	
D. Michael Heinekey	Panelist	University of Washington
	http://depts.washington.edu/chem/people/faculty/heinekey.html	

Heavy Element Chemistry/Separations and Analyses

Carol Burns	Panel Lead	Los Alamos National Lab
	cjb@lanl.gov	
Bruce Chase	Panelist	DuPont
	Bruce.Chase@USA.dupont.com	
Sue Clark	Panelist	Washington State University
	http://www.chem.wsu.edu/people/faculty/s_clark.html	
William Evans	Panelist	University of California, Irvine
	http://www.chem.uci.edu/faculty/wevans/	
Michael Heaven	Panelist	Emory University
	http://www.chemistry.emory.edu/faculty/heaven.html	
Robert Hettich	Panelist	Oak Ridge National Lab
	http://ornl.gov/sci/csd/Staff%20CV/OBMS_Hettich.html	

Geosciences

Ed Stolper	Panel Lead	Caltech
	http://www.gps.caltech.edu/people/ems/profile	
Bob Bodnar	Panelist	Virginia Tech
	http://www.geol.vt.edu/profs/rjb/rjb.html	
Randy Cygan	Panelist	Sandia National Labs
	http://www.sandia.gov/eeselector/gc/gc/rtc.htm	
Lars Stixrude	Panelist	University College London
	http://www.geo.lsa.umich.edu/~stixrude/	
Jim Tyburczy	Panelist	Arizona State
	http://sese.asu.edu/FACULTY/tyburczy	

Biosciences

Elisabeth Gantt	Panel Lead	University of Maryland
	http://www.life.umd.edu/grad/mocb/faculty/gantt.html	
Robert Blankenship	Panelist	Washington University
	http://www.chemistry.wustl.edu/faculty/blankenship	
John Richards	Panelist	Cal Tech
	http://www.cce.caltech.edu/faculty/richards/research.html	
John Shanklin	Panelist	Brookhaven Nat Lab
	http://www.biology.bnl.gov/plantbio/shanklin.html	
Kay Simmons	Panelist	USDA
	kay.simmons@ars.usda.gov	

Appendix B: FINAL COV AGENDA
Basic Energy Sciences Advisory Committee
Committee of Visitors for the
Chemical Sciences, Geosciences, and Biosciences Division
April 22-25, 2008

Tuesday, April 22, 2008				
Time	Activity	Committee Members	Division Staff	Location
6:30 PM	Informal Reception/Cash Bar	All	All	Bailey's
Wednesday, April 23, 2008				
Time	Activity	Committee Members	Division Staff	Location
7:45 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers/Vans	Fairfield Inn Lobby
8:30 AM	Welcome and Charge to the Committee	All	John Hemminger, Chair Basic Energy Sciences Advisory Committee	A-410
8:40 AM	Overview of Basic Energy Sciences and the Chemical Sciences, Geosciences, and Biosciences Division	All	Eric Rohlfing, Acting Director, Office of Basic Energy Sciences	A-410
9:30 AM	University and DOE laboratory review procedures	All	John Miller, Acting Director, Chemical Sciences, Geosciences, and Biosciences Division	A-410
9:50 AM	Solicitations during COV period; Contractors' meetings	All	Michael Casassa, Team Lead for Fundamental Interactions	A-410
10:10 AM	SC Demographic Data Collection	All	Linda Blevins, Office of Science	A-410
10:20 AM	Instructions and schedule	All	Geri Richmond, Chair Committee of Visitors	A-410
10:30 AM	Break and disperse to panel rooms			
10:45 AM	First Read Panel 1 Atomic, Molecular, and Optical Sciences Gas-Phase Chemical Physics	Lineberger Gallagher Johnson Suits Xantheas	Jeff Krause Larry Rahn (detailee) Wade Sisk (detailee)	A-410

10:45 AM	First Read Panel 2 Photochemistry Condensed Phase Chemical Physics	Rosky Echegoyen Fujita Gust Hammes-Schiffer Orlando	Mark Spitler Greg Fiechtner	G-426
10:45 AM	First Read Panel 3 Catalysis	Gates Friend Metiu Ozkan Bare Heinekey	Raul Miranda Paul Maupin Michael Chen (detailee)	E-401
10:45 AM	First Read Panel 4 Heavy Element Chemistry Separations and Analyses	Burns Chase Clark Evans Heaven Hettich	Lester Morss Bill Millman	E-114
10:45 AM	First Read Panel 5 Geosciences	Stolper Bodnar Cygan Stixrude Tyburczy	Nick Woodward Patrick Dobson (detailee)	E-301
10:45 AM	First Read Panel 6 Biosciences	Gantt Blankenship Richards Shanklin Simmons	Rich Greene Bob Stack (detailee)	G-207
12:30 PM	Lunch	All	All	A-410
1:30 PM	Resume First Read Panels	Panels		Panel Rooms
4:30 PM	Meeting between Panel Leads and Chair	Panel Leads and Chair	None	F-403
5:00 PM	Meeting with Chair and BES Senior Management	Chair	Eric Rohlfing, John Miller, Rich Greene, Michael Casassa	F-403
5:30 PM	Return to Hotel	All	Drivers/Vans	A-410
6:30 PM	Cash bar	All	All	Carrabba's Italian Grill
7:00 PM	Dinner for COV and BES Staff	All	All	Carrabba's Italian Grill

Thursday, April 24, 2008				
Time	Activity	Committee Members	Division Staff	Location
7:45 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers/Vans	Fairfield Inn Lobby
8:30 AM	Write First Read Panel Reports	Panels	none	Panel Rooms
11:15 AM	COV Executive Session Panel Lead Reports	All	none	A-410
12:00 PM	Lunch	All		A-410
1:00 PM	<u>Second Read Panel 1</u> Atomic, Molecular, and Optical Sciences Gas-Phase Chemical Physics	Lineberger Heaven Stixrude Richards Bare Fujito	Jeff Krause Larry Rahn (detailee) Wade Sisk (detailee)	A-410
1:00 PM	<u>Second Read Panel 2</u> Photochemistry Condensed Phase Chemical Physics	Rosky Blankenship Bodnar Johnson Clark Ozkan	Mark Spitler Greg Fiechtner	G-426
1:00 PM	<u>Second Read Panel 3</u> Catalysis	Gates Cygan Echegoyen Simmons Chase	Raul Miranda Paul Maupin Michael Chen (detailee)	E-401
1:00 PM	<u>Second Read Panel 4</u> Heavy Element Chemistry Separations and Analyses	Burns Gallagher Tyburczy Shanklin Metiu Orlando	Lester Morss Bill Millman	E-114

1:00 PM	Second Read Panel 5 Geosciences	Stolper Friend Xantheas Heinekey Evans	Nick Woodward Patrick Dobson (detailee)	E-301
1:00 PM	Second Read Panel 6 Biosciences	Gantt Gust Suits Hammes- Schiffer Hettich	Rich Greene Bob Stack (detailee)	G-207
3:30 PM	Merge reports / Formulate points for report	First Read Panels + Second Read Reps	none	Panel Rooms
5:30 PM	Return to hotel	All	Drivers/Vans	A-410
	Dinner on your own	All	None	Local restaurant information provided
Friday, April 25, 2008				
Time	Activity	Committee Members	Division Staff	Location
7:45 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers/Vans	Fairfield Inn Lobby
8:30 AM	COV Executive Session	All	none	A-410
9:15 AM	Closeout Session with COV and BES Senior Management	All	Eric Rohlfing, John Miller	A-410
10:00 AM	Closeout Session with COV and BES Staff	All	All	A-410
10:45 AM	COV Chair meets with Panel Leads	COV Chair Panel Leads	none	A-410
Thank-you!				

Appendix C: FIRST-READ/SECOND-READ/MERGE REPORT TEMPLATE

Panel 1: Atomic, Molecular, and Optical Science and Gas-Phase Chemical Physics

BES COMMITTEE OF VISITORS (COV)
Reviewing the Chemical Sciences, Geosciences, and Biosciences Division
Fiscal Years 2005, 2006, and 2007

Charge to the COV:

I. 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.

II. 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.

III. Assess the program's contribution to progress in achieving the Office Basic Energy Science long term goals (shown in III, below) that are being tracked by the Office of Management and Budget (OMB).

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the programs' processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Consider, for example:

- consistency with priorities and criteria stated in the program's solicitations, announcements, and guidelines
- adequate number of reviewers for balanced review; use of reviewers having appropriate expertise/qualifications; use of a sufficiently broad pool of reviewers; avoidance of conflicts of interest
- efficiency/time to decision
- completeness of documentation making recommendations

Findings:

Comments:

Recommendations:

(b) Monitor active project and programs

Consider, for example

- written progress reports
- contractors meetings
- site visits
- effective interactions between program managers and PIs

Findings:

Comments:

Recommendations:

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) the breadth and depth of portfolio elements

Consider, for example:

- the overall quality of the science
- the balance of projects with respect to innovation, risk, and interdisciplinary research
- the evolution of the portfolio with respect to new investigators and new science thrusts
- the relationship of the portfolio to other parts of the Division and BES
- the relevance of the portfolio with respect to the missions of the program, division, BES, and DOE
- the appropriateness of award scope, size, and duration

Findings:

Comments:

Recommendations:

(b) the national and international standing of the portfolio elements

Consider, for example:

- the uniqueness, significance, and scientific impact of the portfolio
- the stature of the portfolio principal investigators in their fields
- the leadership position of the portfolio in the nation and the world

Findings:

Comments:

Recommendations:

III. PROGRESS TOWARD THE LONG-TERM GOALS OF THE OFFICE OF BASIC ENERGY SCIENCES

In this section the COV should evaluate the program’s contribution to *progress* toward achieving the Office Basic Energy Science long-term goals (shown below) that are being tracked by the Office of Management and Budget (OMB). For each goal, adjectival ratings are defined and a template for rating each goal is provided.

A. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

- Definition of “Excellent” – BES-supported research leads to important discoveries that impact the course of others’ research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries.
- Definition of “Good” – BES-supported research leads to a steady stream of outputs of high quality.
- Definition of “Fair” – BES-supported research leads to modest outputs of good quality.
- Definition of “Poor” – BES-supported research leads to limited outputs.

Progress rating for the program under review (select one):

- Excellent
- Good
- Fair
- Poor

Comments:

B. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and

on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

- Definition of “Excellent” – BES-supported research leads to important discoveries that impact the course of others’ research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries.
- Definition of “Good” – BES-supported research leads to a steady stream of outputs of high quality.
- Definition of “Fair” – BES-supported research leads to modest outputs of good quality.
- Definition of “Poor” – BES-supported research leads to limited outputs.

Progress rating for the program under review (select one):

- Excellent
- Good
- Fair
- Poor

Comments:

C. By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

- Definition of “Excellent” - BES-supported research leads to important discoveries that are rapidly and readily available and feed, as appropriate, into use or projected use by the Department’s technology offices, by other federal agencies, and/or by the private sector. There is evidence of substantive interactions with the Department’s technology offices in most BES program areas.
- Definition of “Good” - BES-supported research leads to a steady stream of outputs of high quality that show the potential to impact energy research.
- Definition of “Fair” – BES-supported research leads to modest outputs of good quality that show the potential to impact energy research.
- Definition of “Poor” – BES-supported research leads to limited outputs that show the potential to impact energy research.
-

Progress rating for the program under review (select one):

- Excellent
- Good
- Fair
- Poor

Comments:

D. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

- Definition of “Excellent” - BES-supported research leads to new concepts and designs for next-generation instruments and detectors for x-ray, neutron, and electron-beam scattering.
- Definition of “Good” - BES-supported research leads to new instruments that are world class.
- Definition of “Fair” – BES-supported research leads to modest outputs of good quality that show the potential to impact the concepts and designs for next generation instrumentations.
- Definition of “Poor” – BES-supported research leads to limited outputs that show the potential to impact the concepts and designs for next generation instrumentations.

Progress rating for the program under review (select one):

Excellent

Good

Fair

Poor

Comments:

Appendix D: FINDINGS, COMMENTS, AND RECOMMENDATIONS OF INDIVIDUAL SUBPANELS

The detailed findings, comments, and recommendations of each subpanel presented below were not discussed by the COV as a whole, although all COV members had the opportunity to read and comment on all of the subpanels' findings and recommendations in their review of the draft COV report. In addition, many of the findings and recommendations common to more than one subpanel were discussed in the COV meeting on Thursday and with CSGB Division Management and Staff on the last morning of the COV meeting.

A. FINDINGS AND RECOMMENDATIONS OF THE AMO SCIENCE/GAS-PHASE CHEMICAL PHYSICS SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the program's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

- Data systems still provide inadequate support
 - Better track demographics, reviewers, pubs, etc
- Quality of decision documentation exceptional
 - Remarkably detailed, thoughtful, and informative
 - Reflects experience and quality of program managers
- Average time to decision under six months
- Flat CSGB funding is producing stress on all programs
 - If it continues, the scope of programs must be reduced to maintain viability
- Initiatives used for innovative and high risk projects
- Remarkable program redirection in AMO
- Internationally recognized investigators/programs

Comments:

The solicitations carried out for the initiatives, such as chemical imaging, have been conducted in a consistent and efficient manner. Requesting white papers, or preproposals, ensured that the investigators who were unlikely to be successful did not waste their time writing proposals and that reviewers were not overwhelmed with so many proposals that they could not do a thorough job of reviewing. While the solicitations for the core programs are broad, as are the programs, we observe that they led to the redirection of the AMOS program, as described in Section IIa.

There were at least four, and more typically five or six reviewers for each proposal, a number which is more than adequate. More important, the reviewers are very knowledgeable and submitted in almost all cases thorough and informative reviews. A point which is particularly noteworthy is the number of excellent European reviewers, which not only provides broader

reviewing expertise but also increases the visibility of the DOE programs. One change in the selection of reviewers could be considered, adding a reviewer who is more of a generalist to assess the broader scientific impact of proposed research. This change could lead to more cohesive programs and more links between programs.

The proposals are processed efficiently. The typical time to decision for the proposals examined was four to five months, and in no case was it as long as one year. It is hard to see how it can be any faster.

Reading the selection memoranda prepared by the program managers was a delightful experience. The expertise and thoroughness with which they were prepared is stunning. The reviewers' comments, both positive and negative, were carefully weighed, and the rationale for inclusion of the proposed work in the program was presented in a clear and convincing fashion.

In a different area, the subpanel wondered whether the EPSCOR programs could be usefully employed to assist in enhancing diversity. We noted the absence of a data base to allow us to effectively engage this issue.

Recommendations:

- Data systems improvement essential
 - Need to track demographics, metrics, productivity, etc.
- Consider adding an "outside the immediate field" reviewer
- Diversity Issues
 - Use data systems to track minority serving institutions as reviewers, proposal submitters
 - EPSCOR opportunity?

(b) Monitor active project and programs

Findings:

- The program managers do an excellent job in managing the research projects and they are handling the renewal process in a timely and efficient manner. This is mainly accomplished by the annual contractors meetings and the site visits to National Laboratories.
- The annual contractor meetings represent the most important and effective vehicle for the program managers to monitor the active programs. The PIs are required to submit an extended (ca. 4 page) abstract for those meetings noting the publications resulted under DOE support and present their results every 3 years. This is a very effective format of increasing and sustaining cross-communication among the PIs funded by the same program. The annual contractor meetings are evolving into premier scientific meetings in their respective fields. We note the efficacy of inviting PIs from other DOE programs to those meetings.
- The site visits to the National Laboratories in the years between reviews are important to the program managers both in monitoring the research programs and informing of new research accomplishments and research directions.
- Due to constraints in the travel budget it is not currently possible for program managers to carry out similar visits to those academic institutions where they support several research programs.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) The breadth and depth of portfolio elements

Findings:

- These programs consistently feature world-leading science, recognized as such.
- The awards given for initiatives in particular show a clear willingness to invest in high-risk, potential breakthrough science. In the core programs this is less clear and perhaps less necessary.
- The GPCP program shows some prudent shifting of priorities and the restructuring with the split of the CPIMS was carried out quite effectively. The elimination of the Chemical Energy and Chemical Engineering program was a wise move to preserve core strengths in a flat budget scenario. The remarkably successful redirection of the AMOS program is a very impressive achievement.
- The GPCP program clearly addresses the DOE mission in combustion research, showing an important mix of disciplines and a range of effort from fundamental reaction dynamics, to kinetics, to flame chemistry, to the chemistry in turbulent flows, with appropriate theoretical input across these scales and powerful experimental techniques. The AMOS program has shown a strong shift to new light sources and the new science they will enable, in part laying the foundation for LCLS.

Comments:

The portfolios show a strong mix of interdisciplinary, world-leading science comprising the core programs to appropriate high-risk responses to the initiatives. The scientific acumen and leadership demonstrated in the reshaping of these portfolios is worthy of recognition.

(b) The national and international standing of the portfolio elements

Findings:

AMO Science has seen a transformation in recent years. It has evolved from a field in which the fundamental interactions of atoms, molecules, photons, and electrons are probed to one in which they are controlled. This control is facilitated by the development and application of novel x-ray light sources and ultrafast probes. AMO Science has provided new ways to control and probe interactions in the gas and condensed phases, which enhances our ability to understand materials of all kinds and makes full use of the BES x-ray sources and Nanoscale Science Research Centers (NSRCs). Synchrotron-based AMO science in the US receives major support from the AMO Science program, and continues its role as the principal US supporter of research into the properties and interactions of atomic and molecular ions relevant to fusion plasmas. Additionally, AMO Science is competitive with Europe and Japan in areas of ultrafast laser science and ultracold molecules.

The Chemical Physics Research program has a far reaching impact on the DOE mission, including energy utilization, catalytic and separation processes, energy storage, and

environmental chemical and transport processes. The Chemical Physics Research program is split into two distinct programs: (1) Gas-Phase Chemical Physics (GPCP) and (2) Condensed Phase and Interfacial Molecular Science (CPIMS). As a result of the GPCP research portfolio, DOE is the principal supporter of high-temperature chemical kinetics and gas-phase chemical reaction dynamics in the nation. Among several national laboratory programs, the GPCP program supports the Combustion Research Facility (CRF), a unique facility that hosts a visitors program for collaborating scientists. It provides strong synergism with the Office of Fossil Energy (FE), the Office of Energy Efficiency and Renewable Energy (EERE) and industry. CPCP plays a leading role in the international combustion research community as evidenced by the large number of papers at the International Combustion Symposium.

National and international recognition of the PIs in these programs include MacArthur, Rabi, Goepfert-Mayer, Davisson-Germer awards, as well as multiple memberships in major honorific groups (National Academy of Sciences, National Academy of Engineering, and the American Academy of Arts and Science).

B. FINDINGS AND RECOMMENDATIONS OF THE PHOTOCHEMISTRY/CONDENSED PHASE CHEMICAL PHYSICS PROGRAMS SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the program's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

- The Panel finds that both the Photochemistry and Condensed Phase Chemical Physics programs handle reviews in very good accord with the programs' priorities and criteria based on published information.
- The funded laboratory programs are manifestly distinguished by the synergy among participants in the funded group and/or by their implementation of unique instrumentation.
- The number of reviews obtained is very good, the reviewers selected are very appropriate, the number of distinct reviewers is large, and there was no evidence of any conflict of interest issues.
- The efficiency and time to decision for rejections appeared generally appropriate (4-8 months), with occasional delays of 1 year or more. It was more difficult to discern the time to approve grants that would be funded, requiring a search through each individual jacket, but it appeared anecdotally longer on average.
- The documentation of recommendations for the Condensed Phase and Interfacial Molecular Science (CPIMS) awards appeared to be very good uniformly. For Photochemistry, it was very good for the most recent awards, but quite erratic for earlier awards (2005-2006).
- Site visit reviews in which each team member writes comments on every aspect of the program reviewed generated considerable redundant and conflicting information and, in some cases, comments that appear to be lacking in expertise.

Comments:

- The Panel was particularly impressed with the level of detail in the reviews provided to the programs, so that the scientific basis for concerns (or praise) could easily be discerned by any reader. At the same time, the individuals selected for the reviews represented quite thoughtful choices.
- The fact that reviewers are not used repeatedly each year, evidenced by the numbers used, serves to retain their involvement in the review process over time.

- The Summaries and Selection Statements provided an excellent digest of the content of reviews, an impressive reflection of the time and effort invested by Program Managers in the process.
- The change in the quality of documentation for the Photochemistry files appears correlated closely with the reorganization of Programs and the new Program Managers, so no corrective action appears to be needed.
- The need to have full reviews from every member of a site visit team is wasteful of effort by reviewers and by those reading the reviews.
- The existence of a convenient database of grants and pending proposals at DOE would be useful to Program managers in examining an applicant's DOE funding portfolio.

Recommendations:

- Both Programs appear to be operating very well under the current organization and leadership. However, it would serve these programs (and the review of these programs) greatly in terms of efficiency and tracking if the information regarding reviewers used, individual reviewer statistics, and process dates were captured in readily accessible form. The Panel urges the implementation of such a database, a fairly standard element of comparable operations at major journals and funding agencies.
- Site visit team reviewers should be encouraged to omit any comments on areas outside of their specific area of expertise, unless they feel confident in their opinions.
- The Panel believes that it is important to use mail reviews as a routine element of site visits to supplement the expertise available in a limited site visit panel.

(b) Monitor active project and programs

Findings:

- The Panel found that annual progress reports were evident in renewal files.
- Contractors meetings provided a very good and consistent means for active monitoring of programs by managers, as well as a good opportunity for interactions between DOE staff and PI's. In addition, these meetings provide an important element of feedback among PI's and stimulate new collaborations.
- The Program managers have encouraged cross-fertilization between areas by including speakers from other programs at each Contractors meeting, contributing to program evolution.
- Site visits to laboratory groups clearly manifest active management by Program managers, with clear delineation of problems, as well as positive accomplishments. In addition, there was evidence that poorly performing elements or programs were addressed by discontinuation if warranted.

Comments:

- The review of the elements of the overall Radiation Science program, identified as needed by the previous COV, was effectively carried out via site visits, with considerable changes implemented to the overall benefit of that research line. In particular, the Notre Dame Radiation Laboratory appeared to be operating at a high level with excellent productivity and new directions under new leadership at the end of 2007.
- The radiation science program at BNL has also improved.
- The fact that all PI's now are associated with an appropriate Contractors meeting is an important positive change which should provide long term benefits.
- The Panel encourages the efforts at cross-fertilization between programs.

Recommendations:

- The Panel recommends, in the strongest terms, the rigorous collection of research impact metrics, facilitated by a comprehensive database of publications, citations, and awards associated with each grant.
- The Panel recommends continuation of other current policies for these programs.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) the breadth and depth of portfolio elements

Findings:

- The Panel found that the rather new CPIMS program was a genuinely excellent development, providing a grouping of projects in close alignment with current scientific thinking and development in both experimental and theoretical areas. It further is now providing a rational placement for the condensed phase dynamics elements of Radiation Science. The result is that these individuals now have a Contractors meeting which provides stimulating interactions and feedback from a relatively broad group of scientists, including leading theoretical groups, and this should provide considerable benefits to both radiation science and more general condensed phase dynamics over time.
- The alignment of Photochemistry with the area of Solar Photochemistry brings the program into focus on one of the major potential solutions to sustainable energy.
- The Panel found that the overall portfolio included a very good range of projects focused on recognized critical fundamental science issues in condensed phase phenomena and photochemical processes.
- The reviews provided evidence that high risk-high impact projects were included in the portfolios, and that routine incremental science projects were not encouraged.

Comments:

- The character of much of the research in these programs reflects the evolution of research into materials synthesis and materials characterization into a truly interdisciplinary effort.

Recommendations:

- The availability of information about the number of grants that are, for example, new, active among young investigators, or terminated, can be discerned by study of the list of individual grants by Program managers, but such data should be readily available in a database. The same is true for data on inclusion of underrepresented groups. This would be very valuable to Program managers, their Division leadership, and the COV.
- The Panel strongly encourages these programs to enhance the representation of women and underrepresented minorities in their portfolios.
- The Panel encourages these programs to continue to enhance the number of new young investigators in their portfolios.

(b) the national and international standing of the portfolio elements**Findings:**

- The Panel found that the individual research proposals supported by the programs represented many of the leading research groups in these areas, based on name recognition of the individuals by Panel members.
- The Solar Photochemistry program encompasses the leading players in the US, and is certainly competitive with any program globally.
- The measures of success for individual programs reported to the COV was based solely on anecdotal data describing, for example, individual notable papers and/or awards, as reported by PI's.

Comments:

- The lack of any quantitative metrics of impact or stature based, for example, on publication records, is a weak point of the Programs which should be remedied.
-

Recommendations:

- Again, the Panel recommends, in the strongest terms, the rigorous collection of research impact metrics, facilitated by a comprehensive database of publications, citations, and awards associated with each grant.

C. FINDINGS AND RECOMMENDATIONS OF THE CATALYSIS SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the program's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

The catalysis program plays a central role in the new opportunities and initiatives throughout the BES portfolio.

Overall, the review and decision-making processes in the Catalysis program are judged to have been excellent. Most reviews were substantive. The number of reviewers was appropriate for balance. The reviewer qualifications on the whole were exemplary, and the expertise of reviewers was well-matched to particular proposals, with international reviewers adding valuable insights. The pool of industrial reviewers is small, and the program would benefit from additional industrial perspectives.

The Program Managers (PM's) exercised sound judgment in making awards and clearly documented the basis for decisions. Time to decision was generally appropriate; decision times were typically approximately 6 months (with a range of 3–11 months).

Documentation was complete, but not easily accessible

Comments:

The review and award process is strong and the management team highly competent, but the process would benefit from improved data management tools.

Recommendations:

A database is recommended to facilitate tracking and understanding of the rationale for funding decisions and for later evaluation of the quality of those decisions. The data bases should include information about reviewer expertise, demographics, and responsiveness, quality, and agreement with other reviewers.

We also recommend a paperless proposal handling system to increase the efficiency of proposal evaluation and enrichment of the pool of industrial reviewers.

(b) Monitor active projects and programs

Findings:

The PM's effectively used contractors meetings and participation in national and international scientific meetings to monitor active projects and programs. Data characterizing research outcomes (e.g., publications, patents, etc.) were not readily accessible for evaluation. Extraction and organization of information for evaluation was done by hand and with great time investment by DOE staff.

Recommendations:

In agreement with prior COV reports, we urge DOE to create an effective data base for proposal management to promote efficiency and excellence. Information important for the monitoring programs includes the following: annual reports, including publications resulting from the projects; citation impact, awards, and patents. Statistical tools should be developed in tandem with the database.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) the breadth and depth of portfolio elements

Catalysis is the cross-cutting discipline most central to the BES mission, as documented in program materials exemplified by the 2003 BESAC report on "Research for a Secure Energy Future." For example, catalysis is important for development of renewable energy sources, energy storage and conversion, transportation, carbon management, and application of hydrogen as a fuel.

The catalysis science initiative, consisting of 11 projects involving teams of investigators from multiple institutions, includes some of the most innovative projects in the program. As the fundamental science supported by BES is increasingly performed at the interfaces between sub-disciplines, the catalysis science initiative might be considered as a model for other BES programs.

The support for the XAFS consortium based at the NSLS is viewed as positive; productivity in terms of publications has increased. The funding has allowed development of a facility that is of benefit to many in the BES catalysis community.

The DOE catalysis program supports a broad portfolio of investigations that are central to the development of new areas in catalysis. The award process has led to a good balance of innovative/high risk research, research with clearly defined outcomes, and tool development. Several superb new investigators at relatively early career stages have been included in the program.

One of the characteristics of the BES catalysis program is its connections with industry. Contractors meetings include industrial participants, and there are collaborations between industrial researchers and PI's supported in the DOE catalysis program.

The scope of awards is generally appropriate; however, the impact and effectiveness of awards is being eroded by the increasing cost of research.

Timely, merit-based extension of funding for selected strong programs for 1-2 years should be considered at the discretion of the PM's.

(b) national and international standing of the portfolio elements

Findings:

The Catalysis program funds highly recognized and high-impact researchers.

PI's in this program have received numerous awards for DOE-funded work, including numerous ACS National Awards, a Nobel Prize, and several major international awards.

Recommendations:

The PM's should continue to evaluate the quality and achievements of program research and solicit new ideas for high-risk work with high potential for future impact.

D. FINDINGS AND RECOMMENDATIONS OF THE HEAVY ELEMENT CHEMISTRY/ SEPARATIONS AND ANALYSIS SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the program's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

- (1) Overall, our impressions of solicitation, review, recommendation, and documentation of portfolios were very favorable. The panel recognized that we were reviewing two types of awards – contracts to laboratories and grants to universities. We judge that the effort made to more widely acquaint the community with open announcements through such mechanisms as “Dear Colleague” letters has been successful.
- (2) The preproposal process utilized for the initiatives is very useful mechanism, saving everyone (proposers and program staff) time.
- (3) We saw a very good selection of reviewers, and in nearly all cases felt program staff had worked hard to ensure an adequate and equitable number of reviews. No information was available, however, on “diversity” of reviewers (age, experience, gender, etc); we do not believe this information is tracked.
- (4) The range of times from receipt of proposal to the award decisions is (usually) 6 months to (at times) 12 months. Although some of the longer decision times appear to be associated with funding uncertainty (transition over fiscal year boundaries), overall we believe performance has improved in this area. It would be beneficial to establish and advertise a target time period for review, i.e. 80% of proposals reviewed and responded to within six months.
- (5) The depth and quality of the reviews, and the responsiveness of the reviewers are excellent (the personal attention and subject matter knowledge of the program managers is an important factor here).
- (6) For the marginal decisions, we elicited additional information on how these decisions were made (e.g. why was the opportunity for response provided to some proposers, but not to others). We felt the decision making process was sound in all cases, but that further information on this decision-making should be included in the files.
- (7) The process for evaluating laboratory-based programs is still not entirely transparent in the marginal cases, probably due to the complexity of the interface with lab management in contract management. While progress has been made in focusing lab reviews on proposed work, there is still an emphasis on past achievements as opposed to proposed research.

Comments

- (1) For the Heavy Element Chemistry program, the solicitation of proposals (with respect to other portfolios) has been limited by the cancellation of the ANES call (the most relevant initiative to this portion of the portfolio). Consequently, only limited progress has been made in identifying new researchers (only one new academic

portfolio). In the period reviewed nine proposals for the core program were declined. However, 118 full proposals were submitted in response to the ANES call (61 in the combined separations and analysis and HEC area), indicating that the proposal pressure in this area is much greater than indicated by the data for the core program alone. Clearly, the size of the portfolio cannot accommodate new starts without new funds.

Recommendations:

- (1) Collect information on reviewers: institution, BES funded/non-funded, frequency of use, response time, demographics, etc. for inclusion in an information management system to facilitate identification of reviewers, and to ensure equity is considered in the selection of reviewers.
- (2) Improve guidance to reviewers; in some cases, specific recommendations from reviewers were not apparent. Consider mandating “summary statements” from reviewers, and requesting clear statements of strengths and weaknesses.
- (3) Direct reviewers for on-site review of national laboratory programs to focus their attention on “forward-looking” proposed science in addition to capabilities of the researchers (as reflected in their accomplishments). Although a shift has been noted in recent reviews, program managers must also enforce this message with laboratory management to continue this progress.
- (4) The continued use of anonymous supplemental mail reviews for laboratory programs is encouraged.
- (5) Improve consistency of documentation and include more information on decisions at the margin (good thinking exists, but isn’t documented).
- (6) Consider advertising target timelines for proposal review/response (80% complete in 6 months).
- (7) We urge an emphasis on chartering the on-site review committees to focus further on work to be done, rather than accomplishments. We suggest an equal weight on evaluation of work accomplished in the previous program period and proposed research plans for the next period. We like the idea of supplemental mail review, and encourage its use.
- (8) We also encourage the consistent use of summary statements and clear statements of strengths and weaknesses from reviewers to facilitate actions by the program managers.

(b) Monitor active project and programs

Findings:

- (1) Primary monitoring of projects occurs through contractor meetings (separations and heavy element chemistry conduct a joint contractor meeting every 2 years, and the analysis portfolio has a separate contractor meeting alternate years), as well as through requests for information (annual reporting, collecting highlights).
- (2) Program managers have the ability to attend a select number of professional society and related technical meetings. The international nature of work associated with heavy element chemistry mandates that occasional travel to international meetings is

necessary. We believe that participation in these meetings contributes to the expertise of the program managers and their technical connection with the community.

- (3) Contractor meetings do include non-funded participants (effort is made to avoid the perception of “pre-selection”); we support this mechanism as a way to educate potential new PI’s and interject new science ideas into the discussion of the programs.
- (4) Information on accomplishments and highlights is maintained electronically by program managers; this probably means that consolidation of this information (and generation of reports to the Office) is more time-intensive for program managers than necessary.
- (5) The project folders generally are not used to retain information on the monitoring of the projects, however, except when a report of accomplishments is provided as part of a renewal proposal. The folders emphasize selection, not monitoring, and as a consequence we weren’t able to evaluate how information collected from PI’s over the course of the project is used in decision making.

Comments:

Recommendations:

- (1) Give “best in class” program managers “best in class” tools – information management systems. Collect information on projects: new investigators to DOE/program, publications, patents, presentations, awards, commercialization successes, new collaborations, annual reports/abstracts from contractors meeting, personnel on project, “nuggets”, information on PI (institution, demographics) number of years funded, funding profile. This will facilitate monitoring of projects and the ability to quickly collect important statistics for internal and external use.
- (2) Include information collected on monitoring the proposals (abstracts from contractor meetings, annual reports, “nuggets”, etc.) in the proposal folders as a point of collection for this information until such time as a database can be created.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) the breadth and depth of portfolio elements

Findings:

- (1) The panel judges that significant progress has been made over the course of the review period in “modernizing” the separations portion of the separations and analysis program.
- (2) The quality of the science in the separations and analysis program is cutting edge; it is judged to be at a level comparable to (and in some cases better) than that supported by other sponsors of fundamental science.
- (3) In the heavy element chemistry portfolio, the panel believes that the overall program is very strong and broad, but the academic portion of the program is “eclectic”, and

not as broadly founded. As previously outlined, this is an artifact of the limited funds of the portfolio, rather than the interest by potential PI's, given that a large number of proposals were received in this area in response to the Advanced Nuclear Energy Systems Initiative (36 full proposals submitted in the actinides and fission products area – this indicates strong proposal pressure).

- (4) The impact of the portfolio was also discussed in the context of specific examples of the translation of research to development within the Department of Energy. We felt that some good examples were presented (development of separations technologies, understanding of actinide behavior in the environment); these accomplishments should continue to be featured (and perhaps more credit should be taken) by program managers and by the Office.
- (5) When asked, the program managers suggested that perhaps 10% of their portfolios can be considered “high-risk” research; we judge this to be an appropriate level.

Comments:

Recommendations:

- (1) We would recommend that some means be identified to capture some of the scientific interest generated by the ANES initiative to improve the breadth of the academic portfolio in Heavy Element Chemistry through introduction of new participants, perhaps through new initiatives (i.e. new money, not a reallocation of resources from within the portfolio).

(b) the national and international standing of the portfolio elements

Findings:

- (1) In the combination of national laboratory and university programs, the quality of work in the Heavy Element Chemistry program is world-class (particularly leading in the application of modern scientific tools in the investigation of the actinides). Evidence exists in the form of participation in (and leadership of) major international conferences, publications in leading journals, and participation of funded investigators on national and international advisory boards.
- (2) The work in the Separations and Analysis portfolio is clearly on par with the best programs nationally and internationally as evidenced by the quality and quantity of publications, the innovative nature of the proposed research, and the participation of the PIs in both national and international conferences, meetings and workshops.

Comments:

Recommendations:

- (1) Owing to the international nature of the heavy element science field, we recommend continued engagement of program management with international specialists in this field, both to ensure the most qualified pool of reviewers for proposals, and to facilitate collaboration between U.S. and international scientists.

E. FINDINGS AND RECOMMENDATIONS OF THE GEOSCIENCES SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the program's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) The processes used to solicit, review, recommend, and document proposal actions within the Geosciences Program are consistent with the program solicitation (in DE-PS02-07ER07-01), and with priorities established within DOE and by the broader community of scientists, as communicated in BES-sponsored workshops and reports (for example, Basic Research Needs for Geosciences 2007) and National Academy reports.

(2) Criteria for evaluation of proposals are clear and are provided to reviewers. The program manager obtained a sufficient number of reviews for each proposal (636 reviews for 215 proposals over the three-year period review). Reviewers had necessary, appropriate, and diverse areas of expertise.

(3) Time-to-decision ranged from three months to over a year. National lab contracts were awarded on an annual cycle (proposals received in January, decisions made in June), which generally resulted in a consistent and acceptable time-to-decision. University proposals were evaluated as received, but funding decisions were sometimes affected by timing of congressional appropriations bill. Decisions were typically made within 6-8 months, but exceptions occurred.

(4) Documentation of the rationale and processes behind the decisions is reasonable and appropriate. The memos from the program manager to the director describing each decision were thorough and thoughtful. The program manager used a range of appropriate criteria to maintain a balanced portfolio of funded projects. Reviewer comments were provided to PIs of declined university proposals. Reviews of laboratory proposals are sent to program managers at the laboratory.

Comments:

(1) The second-read panel noted the very positive findings listed above are a compliment to the program manager.

Recommendations:

As recommended in the 2005 COV report, and reiterated in this report, software tools and databases should be developed to track the funding portfolio, the demographics of proposers and reviewers, the funding histories of the investigators, and the products of the grants (journal articles, workshops, etc.). Data to quantify output, effectiveness, and impact of the sponsored research should be developed. A BES-wide database of peer-reviewed publications should also be developed and maintained.

(b) Monitor active projects and programs

Findings:

(1) The Geosciences Program monitors active research projects and related programs through annual progress reports (abstracts of which are collected into a widely distributed document) and through symposia and workshops. Recent symposia focused on analytical and isotope geochemistry (June 2005) and computational and numerical geosciences (May 2007). In addition, the Geosciences Program organized a workshop entitled “Basic Research Needs for the Geosciences: Facilitating 21st Century Energy Systems” (July 2007) that brought together funded PIs and other geoscientists to identify the critical needs in geosciences research as related to DOE goals.

(2) The Geosciences Program sponsored the popular Mineralogical Society of America and Geochemical Society short courses and the resulting publications. Six short course volumes (Reviews in Mineralogy and Geochemistry, RIMG) were produced during 2005-2007 and include *Molecular Geomicrobiology* RIMG vol. 59 (2005), *Water in Nominally Anhydrous Minerals*, vol. 62 (2006), *Neutron Scattering in Earth Sciences* vol. 63 (2006), *Medical Mineralogy and Geochemistry* vol. 64 (2006), *Fluid-Fluid Interactions* vol. 65 (2007), and *Paleoaltimetry: Geochemical and Thermodynamic Approaches* vol. 66 (2007). The program supported a special issue of the geosciences magazine *Elements* and provided funding for several society meetings and special society symposia. These outreach efforts help to highlight the DOE-supported activities within the broader geosciences community.

Recommendations:

(1) As emphasized by the 2005 COV review of the Geosciences Program, we recognize the need to monitor the review history, productivity, output (journal articles, symposia, workshops, citations, etc.), and demographics of the project and its investigators. To quote directly from the 2005 COV report: “Metrics also need to be developed and monitored so that the success and impact of funded research can be evaluated by future Committees of Visitors and within the DOE. Suggested criteria for these metrics include: (i) published papers; (ii) citation impact and frequency; (iii) sponsored workshops and symposia; (iv) use of DOE facilities by the projects; and (v) particularly notable discoveries made as a result of funding by the program. Implementation should not be delayed and need not wait for the development of an elaborate software package; if necessary, it could be accomplished with in-house software using a simple database.” This effort should be given high priority.

(2) A reference database of peer-reviewed journal articles resulting from support of the Geosciences Program should be maintained. Such a compilation would be useful to the program as a supplemental monitoring tool, and would provide documentation of the success, impact, and breadth of the Geosciences Program.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) The breadth and depth of portfolio elements

Findings:

(1) The Geosciences Program has a broad scientific reach and supports research that spans many geosciences disciplines. Supported projects involve topics as diverse as experimental and theoretical geochemistry, biomineralization, rock mechanics, and imaging techniques that span the range from the nano- to lithospheric scales (10^{-9} to 10^6 m).

(2) The overall quality of research projects in the geosciences portfolio appears to be high, but objective evaluation of the quality is difficult without a set of metrics.

(3) The program supports a good mix of high risk projects with high potential payoff as well as lower risk projects required to advance the science.

(4) Interdisciplinary research is an integral component of both university and national laboratory projects. The program supports a good blend of research in biochemistry, environmental science, and materials research including geosciences representation in division-wide initiatives such as Chemical Imaging. A major strength of the Geosciences Program is that it brings together researchers with diverse backgrounds and expertise to address complex problems and includes PIs from other disciplines. Publications are often in journals in fields other than geosciences.

(5) Over the three year period of the COV examination, the program has had about 15% annual turnover in projects and investigators. Turnover of this sort provides new opportunities and is a sign of a healthy program.

(6) The geosciences portfolio addresses scientific challenges articulated by the program manager and presented to the review committee and is consistent with division-wide grand challenges.

(7) Awards in the Geosciences Program are sufficient for the research and project duration is long enough to accomplish research goals. The philosophy of long-term support for successful programs allows PIs to manage graduate student and post doc involvement and to develop long-range research plans. The support of new investigators at national laboratories by individual

grants rather than by a block grant serves to develop the next generation of national laboratory researchers.

Recommendations:

(1) Full assessment of the quality of research supported by the Geosciences Program requires metrics to evaluate quantitatively the research products. These may include but should not be limited to journal impact factors, citations of BES-supported publications, leadership in symposia, and other professional activities, etc.

(2) The success of many DOE mission-critical programs requires significant involvement of earth scientists. We envision the world-class Geosciences Program of BES as the focus of these interactions. The breadth and depth of fundamental research in the Geosciences Program offers opportunities for other DOE programs including those within the Office of Science (e.g., BER). For example, we encourage scientists from other BES programs to participate in the geosciences workshops (contractor meetings). As another example, the applied efforts in CO₂ sequestration being undertaken by the Office of Fossil Energy would be strengthened by additional interactions with BES geoscientists conducting fundamental research addressing this problem.

(3) The Geosciences Program would benefit from having a standing external advisory board or panel with expertise in the various areas supported by the program in order to advise the program manager.

(b) National and international standing of the portfolio elements

Findings:

(1) DOE-supported analytical facilities in geosciences offer distinctive state-of-the-art analytical tools.

(2) Although in the opinion of the COV the portfolio is excellent, influential, and has internationally recognized impact, this is a subjective judgment. However, as emphasized previously, the significance and impact of the program could be better judged if quantitative metrics of the contributions of the work that it supports were available.

(3) The relatively stable funding provided by DOE can provide a strong basis for career development, for risk taking, and for significant contributions. The program has a consistent record of supporting both early career researchers (~15% of the current PIs are less than 10 years beyond their Ph.D.) and more established researchers.

Recommendations:

Again, the COV urges that objective metrics for evaluating the quality, innovation, and impact of the portfolio be implemented.

F. FINDINGS AND RECOMMENDATIONS OF THE BIOSCIENCES SUBPANEL

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the programs's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions

Findings:

- (1) Timely solicitation for proposal from the science community has been effectively continued and has resulted in applications from both young and experienced scientists.
- (2) The two-part review process i.e. of pre-, and full proposals has entailed extensive internal screening, yielding well-developed full investigator proposals in areas appropriate to the mission of the program.
- (3) Examination of the jackets of proposals that were funded or declined shows outstanding compliance to the process. Each proposal was reviewed by about six experts including panel and mail reviewers.
- (4) The program has taken the lead in experimenting with the use of *virtual panel review* via teleconferencing.

Comments:

- (1) The sub-panel was unanimously impressed by the thoroughness, completeness and documentation of the review process.
- (2) The efficiency of using the pre-proposal screening lessens the workload of the reviewers and is endorsed.
- (3) The program is beginning to achieve a balance of grants from young investigators and from those who have been funded over the long term. This achievement is especially commendable in a period of flat funding.
- (4) While participants acknowledge improved efficiency of the *virtual panel review* process, they were not convinced that it is superior to conventional face-to-face panel review.
- (5) Many *Energy Biosciences* research projects would benefit from access to cutting-edge instrumental infrastructure.

Recommendations:

- (1) It is recommended that seed funding be made available to convene a consortium of a group of scientists to assess the interest and needs to integrate increased adoption of biophysical techniques. This could significantly advance research in many phases of the plant and microbial community, with a primary example being a dedicated beam line. A dedicated facility could begin transformational investigations of energy relevant biosystems.

- (2) The process used by the *Energy Biosciences Research* program, of pre-proposals, panel reviews and mail reviews, is highly commendable and should be continued as is.
- (3) In order to more accurately reflect success rates it is recommended that award percentages should be reported on the basis of pre-proposals.
- (4) Before considering adoption of the virtual panel review process, further modifications need to be considered in order not to diminish the review process.

(b) Monitor active project and programs

Findings:

- (1) Three years ago the program was searching for strengths and focus. The previous COV concluded: “Because of the need to appoint new Program Managers in the *Energy Biosciences* program, the Division should take this opportunity to reevaluate and refocus this program in accord with the overall directions and mission priorities of BES and the Division.”
- (2) The sub-panel notes that the program has successfully identified long-term objectives in *Photo- and Bio-Chemistry, i.e., Solar Photochemistry, Photosynthetic Systems, and Physical Biosciences* that define a strong, essential program. The program has identified thrusts that advance key issues, toward a unique and timely program that significantly contributes to the DOE mission area. The panel credits Richard Greene, the new Program Leader, with advancing new focus areas. It is envisioned that the application of innovative physical techniques will strongly enhance energy related studies in plant and microbial systems.
- (3) A strong and successful effort has been made in more fully integrating the program with other programs under BES, especially the physical and chemical sciences, with a positive trajectory of continuing in this direction.

Comments:

The bringing together of the *Solar Photochemistry* program with the *Photosynthetic Systems and Physical Biosciences* programs under the new Photo- and Bio- Chemistry umbrella is a highly desirable development that will facilitate integration between these three programs.

Recommendations:

- (1) Recent retirements that led to inadequate staffing have placed the program at potential risk. The addition of two new Program Managers for this program is essential.
- (2) The emphasis and fuller integration with basic energy sciences should continue. The program should maintain its past and continuing strengths in plant and microbial biosciences.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Findings:

- (1) The quality of science is superb.

- (2) *Energy Biosciences* has had great success in funding fundamental research that has evolved into central themes in plant and microbial biology.
- (3) As recommended by the 2005 COV, *Energy Biosciences* identified mechanisms for co-funding between different BES programs. Co-funding examples are: (a) of the work of Yeung (Ames Laboratory) with the *Catalysis Science Program*, and (b) Arnold (Caltech) with the *Analysis and Separation Program*.

Recommendations:

- (1) *The Photo- and Bio-Chemistry Program* represents the realization of the refocusing of the former *Energy Biosciences* program. We fully endorse the new direction and hiring of 2 new program managers that is in progress.

(b) The national and international standing of the portfolio elements

Findings:

- (1) *The Photo- and Bio-Chemistry Program* is a major funding stream for fundamental research of world-class quality in the plant and microbial sciences.
- (2) *The Photo- and Bio-Chemistry Program* is unique and consists of program elements in large part not funded by NIH, NSF or USDA.
- (3) Over the lifetime of the *Energy Biosciences* program more than 25 scientists have been funded who have subsequently been elected to the NAS. This includes seven newly elected members in the past three years, since the last COV report.

Appendix E: SUBPANEL RATINGS OF PROGRESS TOWARD LONG-TERM BES GOALS

A. Rating of Atomic, Molecular, Optical Sciences and Gas-Phase Chemical Physics Programs

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Progress rating for the program under review (select one): Excellent

Justification: A number of projects supported by these two programs are making direct contributions to the achievement and characterization of new materials and new states of matter. Given the current budget limitations, progress is fully consistent with the stated 2015 goals.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Progress rating for the program under review (select one): Excellent

Justification: A substantial number of projects supported in this program are directed toward controlling matter at the quantum level using light pulses and toward the full characterization of chemical reaction dynamics and energy flow. The supported programs encompass a very healthy mix of theory, simulation and experiment. The projects are of extremely high quality. Given the current budget limitations, progress is fully consistent with the stated 2015 goals.

c. By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Progress rating for the program under review (select one): Excellent

Justification: A substantial number of projects supported in this program have been undertaken by investigators who either wrote portions of the 2003 BESAC Research Needs Report, or whose research is guided in directions consistent with these broad objectives. Given the demonstrated high quality of the investigators, there is every reason to expect significant progress toward radical new concepts by 2015.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review (select one): Excellent

Justification: A substantial number of projects supported in this program are directed toward development of completely new instruments and approach to characterize new materials and to control their behavior. The projects are of extremely high quality. The investigators are developing increasingly more sophisticated and effective methods to shape laser pulses to better control matter. Given the current budget limitations, progress is fully consistent with the stated 2015 goals.

B. Rating of the Photochemistry and Condensed Phase Chemical Physics Research Programs

- a. **By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.**

Progress rating for the program under review (select one): Excellent

Comments:

Both Programs considered here are very well focused on frontier issues of materials assembly and characterization covering a wide range of potential combinations of components and scales, all of potential direct relevance to long term energy-related applications.

- b. **By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.**

Progress rating for the program under review (select one): Excellent

Comments:

- The programs from both theory and experiment focus extremely well on developing the needed science to understand and hence control chemical dynamics in the condensed phase and in complex assemblies.

- c. **By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.**

Progress rating for the program under review (select one): Excellent

Comments:

- The programs from both theory and experiment focus well on developing the science needed to underpin the projected development of the new materials and processes required to access sustainable energy sources.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review (select one): Excellent

Comments:

- The measurements being carried out by the PI's in both programs represent developments at the frontiers in both spatial and temporal resolution, as required for progress toward these goals.

C. Rating of the Catalysis Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Excellent. The PI's in the catalysis program have been leaders in fabricating, characterizing, and analyzing new materials for catalysis applications. A few specific examples are the synthesis of materials that mesoporous, nanostructured, and reactive—in conjunction with creative use of new characterization tools.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Excellent. The program has led to substantial progress in understanding and controlling reactivity for energy-related catalysis in solution, at interfaces, and on surfaces.

c. 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Excellent. The program has generated numerous successes in innovative approaches and methods for creating new materials characterization methods and approaches for controlling chemical transformations. The developments of new methods have driven innovations in energy research. Examples are chemical imaging efforts; grazing-angle X-ray scattering work, and synchrotron and complementary investigations of catalysts under operating conditions.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Excellent. PI's in the DOE Catalysis program have made wide use of instrumentation facilities for catalyst characterization and investigations of processes under operating conditions. For example, the program supports a beamline at NSLS that is dedicated to catalysis research.

D. Rating of the Heavy Element Chemistry and Separations and Analysis Programs

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Progress rating for the program under review (select one): Excellent

Comments: Separations and Analysis (S&A) is a prime example of “enabling technology development”. These programs develop cutting-edge characterization and analysis tools which enable other branches of the Division of Chemical Sciences, Geosciences and Biosciences to effectively evaluate the synthesis and assembly of materials for energy related applications. We found that the principal investigators funded by these programs are among the very best both nationally and internationally. Research being conducted is of outstanding quality and is making highly significant contributions to the knowledge base and understanding of areas of importance to the DOE mission. The Heavy Element chemistry portfolio, while addressing a narrower range of interests, has made strides in incorporating the design, modeling, characterization, and assembly of new materials and structures to meet priority needs stated for the portfolio. The programs funded by HEC have no other obvious sources of federal support. It is critical for the DOE and for the nation that these programs continue to flourish. These programs have a history of excellence, having provided unique resources for other investigators and supporting scientists who have received some national and international recognition. However, at present, the number of supported programs and new investigators being added to the contractor pool is below critical needs for HEC.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Progress rating for the program under review (select one): Excellent

Comments: As stated in part A, programs in HEC and S&A are playing critical roles in providing novel enabling technology. Some of the programs in chemical imaging

contribute directly to the understanding of chemical reactivity and energy transfer at surfaces and nanostructures.

c. By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Progress rating for the program under review (select one): Excellent

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review (select one): Excellent

Comments: Much of the work currently supported by S&A is directed towards the development of characterization tools which can then be used in the development of new materials and as a part of potential process control instrumentation. In the heavy element area there has been outstanding work on the characterization of actinide compounds and their solvation environments at the user facilities at ANL and LBNL.

E. Rating of the Geosciences Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Geosciences Program Rating (A): Excellent

Justification of Rating:

Research being conducted in the Geosciences Program is at the leading edge in modeling, characterizing, and analyzing a variety of complex new materials and structures including synthetic and natural nanomaterials, biomaterials, ceramics, glasses, melts, fluids, interfaces, and surfaces that may have energy-related applications. Geoscientists are positioned and experienced to make progress in these areas at both the fundamental and applied levels. Moreover, the Earth's crust, from which most energy resources are extracted, is itself a complex heterogeneous material with properties that must be understood over many length scales. The challenges of studying these systems are being met through the BES Geosciences Program.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Geosciences Program Rating (B): Excellent

Justification of Rating:

A major focus of the Geosciences Program is understanding of complex interfacial processes, many of which are important for characterizing and modeling processes in the subsurface including carbon sequestration, waste isolation, and other energy-related applications. As a result of geochemical processes, the Earth is a source of a wide variety of natural compounds, often with novel and unexpected properties. Lessons learned from characterization and understanding of these systems will continue to have important impact on our understanding of chemical reactivity in energy applications.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Geosciences Program Rating (C): Excellent

Justification of Rating:

Studies of earth materials have influenced development of fuel cells, catalysts, solar cells and other materials. Most energy sources are derived from the Earth and often byproducts of energy production often require long-term subsurface storage. Advances in mineral physics, geomaterials characterization, imaging from atomic to crystal scales, and understanding the fundamental molecular interactions between rocks and fluids are critical to these developments.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Geosciences Program Rating : Excellent

Justification of Rating:

Geoscientists have been leaders in the development and application of synchrotron facilities such as the Advanced Photon Source, the Advanced Light Source, the National Synchrotron Light Source, and the Stanford Synchrotron Radiation Laboratory. Dedicated beamlines at these unique facilities, including the GeoSoilEnviro Consortium for Advanced Radiation Sources (GSECARS), have been successful at characterizing chemical composition at the atomic scale as well as structure and bonding.

Geoscientists were among the first to use the Spallation Neutron Source for characterization of the structure of compounds with light elements, such as hydrogen, and the magnetic structure of materials.

Research supported by the Geosciences Program involves innovations in microanalytical techniques such as nano-SIMS, multicollector ICP-MS, scanning tunneling and atomic force microscopy, and other methods.

Advanced computation has had a major impact on molecular modeling of materials at increasing levels of complexity and accuracy, and subsurface characterization via inversion of surface seismic and potential field measurements for in situ earth structure

F. Rating of Biosciences Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Progress rating for the program under review: Excellent

Justification. Representative examples are: Elliot Meyerowitz (CalTech) made progress in dissecting the flowering pathway in Arabidopsis by discovering a key transcription factor (LEAFY). In Mark Estelle's (Indiana University) pioneering work on plant hormone action he discovered a family of five auxin receptors that are responsible for directing the degradation of negative regulators of hormone action, thus activating transcription. Chris Somerville's team (Carnegie Institute of Washington/Stanford) developed a real-time fluorescence method for observation of the biosynthesis of cellulose, and used the system to characterize the molecular and cellular mechanisms governing cellulose biosynthesis.

The two collaborative projects, PRL (Michigan State) and CCRC (University of Georgia) continue their excellence. In addition to their unique training roles (in the plant molecular biology and carbohydrate areas), original research contributions flow from these investigators. Two examples of many, are Marcus Pauly who made the successful transition from Germany to Michigan, and Alan Daryll at CCRC who, in various complementary ways, explore the role of hemicelluloses and pectins in plant growth and development.

Another significant program at the PRL is that of Rob Larkin, whose group studies chlorophyll biosynthesis as well as plastid signals that have a profound effect on chloroplast biogenesis and photomorphogenesis.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Progress rating for the program under review: Excellent

Justification: Research from Michael Adams (University of Georgia) furthers our understanding of the novel energy transduction processes of hyperthermophilic Archaea. These primitive organisms produce hydrogen using unique thermally stable enzymes. New mechanisms of carbon dioxide fixation have been discovered recently by John Peters (Montana State University). These mechanisms may have utility in devising new methods for carbon sequestration based on biomimetic chemistry. A. Portis (USDA-ARS, Illinois), has modified the key photosynthesis enzyme, RUBISCO, and determined how the enzyme can be altered to remain active under high temperatures, which increases photosynthetic efficiency and crop yield when field temperatures rise, conditions that would normally result in lowered RUBISCO activity. Robert J. Spreitzer (U. of Nebraska) discovered how altering the small subunit of RUBISCO can increase enzyme activity paving the way for plant scientists to increase tolerance to heat stress and maximize photosynthetic yield.

c. By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Progress rating for the program under review (select one): Excellent

Justification: The recent discovery of a sixth group of phototrophic bacteria by Donald Bryant (Penn State University) is an exciting development that expands our knowledge of the universe of organisms that can do photosynthesis and helps to define the universal aspects of this critical process. The work of Vittal Yachandra and Kenneth Sauer (LBNL) on structural determination of the manganese (Mn) site of the oxygen evolution complex of plants has brought a new level of structural and mechanistic detail to this most difficult chemical step in the process of water splitting into hydrogen and oxygen. A deep understanding of this chemical process is key to the goal of artificial photosynthesis and is the focus of many bio-mimetic efforts around the world. A pioneering advance in understanding physical processes that underlie photosynthetic energy transfer was made recently in a collaboration between two teams of investigators supported by different BES programs. Graham Fleming (LBNL) and Robert Blankenship (Washington University) used two-dimensional laser spectroscopic analysis of an antenna complex isolated from a photosynthetic bacterium to reveal previously unknown quantum coherence processes.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review: Good

Justification: The last (2005) COV review deemed this category “not applicable,” there was no project that had a significant component of instrumental development. This year presents a happily different situation that follows from the new focus on “physical biosciences.” Three newly funded programs document this comment.

Moerner, W. E. (Stanford) is using an anti-Brownian electro-kinetic trap (ABEL), including a time-correlated single photon counting device, that records the arrival time of all detected photons to study single molecules of a photosynthetic antenna protein (allophycocyanin). This protein captures photons and funnels the energy into the photosynthetic reaction center. This work is at the forefront of single molecule studies of a system that has a fundamental role in harvesting the sun's energy for photosynthesis.

Ackerman, Eric (PNNL) uses single molecule imaging, controlled electrochemical potential and nanoscale confinement to measure and to optimize the properties of redox enzymes. Oxidation/reduction plays a central role in energy generation and flow in all of biology. Ackerman's proposal brings very innovative physical techniques to gain fundamental insights into these processes. It also has the potential to allow the engineering of more effective redox proteins.

Ogilvie, Jennifer (University of Michigan) uses the newly developed method of two-dimensional spectroscopy to gain unique insights into light-harvesting complexes in purple photosynthetic bacteria. These three examples illustrate new directions in physical biosciences that promise great rewards and are being undertaken by investigators with excellent prior accomplishments, two of whom are young investigators.

Whereas it is too early to rate the outcome of these programs, it is appropriate to rate Rich Greene's decision to support these innovative studies in Physical Biosciences as EXCELLENT.



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October 4, 2007

Professor Geraldine Richmond
Richard M. and Patricia H. Noyes Professor
Department of Chemistry
212 Willamette Hall
1253 University of Oregon
Eugene, OR 97403-1253

Dear Professor Richmond:

The Basic Energy Sciences Advisory Committee (BESAC) has been charged by the Department of Energy Office of Science to assemble a Committee of Visitors (COV) to review the management processes for the Chemical Sciences, Geosciences, and Biosciences Division of the Basic Energy Sciences (BES) program. Thank you for agreeing to chair this BESAC COV panel. Under 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.

The panel should assess the operations of the Division's programs during the fiscal years 2005, 2006, and 2007. The panel may examine any files from 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) Photochemistry and Radiation Research
- (4) Catalysis and Chemical Transformations
- (5) Separations and Analyses
- (6) Heavy Element Chemistry
- (7) Chemical Engineering and Chemical Energy
- (8) Geosciences Research
- (9) Energy Biosciences

You will be provided with background material on these program elements prior to the meeting. The COV is scheduled to take place on April 23-25, 2008 at the BES/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A presentation to BESAC is requested at its Summer 2008 meeting (as yet unscheduled). Following acceptance of the report by the full BESAC committee, the COV report with findings and recommendations will be presented to the Director of the Office of Science.

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 projects 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.

In addition to the above elements, the panel is asked to provide input for the Office of Management and Budget (OMB) evaluation of Basic Energy Sciences progress toward the long-term goals specified in the OMB Program Assessment Rating Tool (PART, attached). Each of the nine components (or sub-components, if appropriate) of the Chemical Sciences, Geosciences, and Biosciences Division should be evaluated against each of the four PART long-term goals. If a particular long-term goal is not applicable to a specific program component, please indicate so in the evaluation. Note that the OMB guidelines specify ratings of (1) excellent, (2) good, (3) fair, (4) poor or (5) not applicable. In addition to these ratings, comments on observed strengths or deficiencies in any component or sub-component of the Division's portfolio, and suggestions for improvement, would be very valuable.

If you have any questions regarding BESAC or its legalities, please contact Karen Talamini, Office of Basic Energy Sciences at 301-903-4563 or by e-mail at karen.talamini@science.doe.gov. Diane Marceau, the Program Analyst for the Chemical Sciences, Geosciences, and Biosciences Division, will provide logistical support for the COV meeting. She may be contacted by phone at 301-903-0235 or by e-mail at diane.marceau@science.doe.gov. For questions related to the Chemical Sciences, Geosciences, and Biosciences Division, please contact Eric Rohlfiing, 301-903-8165, or by e-mail at eric.rohlfing@science.doe.gov. Also, if I can be of any help with the process, please feel free to contact me, 949-824-6020 or by email at jchemmin@uci.edu.

Sincerely,

John C. Hemminger, Chair
Basic Energy Sciences Advisory Committee

Attachment

cc: P. Dehmer
E. Rohlfiing
K. Talamini
D. Marceau

**Office of Management and Budget
Program Assessment Rating Tool (PART)
Long Term Measures for DOE Basic Energy Sciences**

- By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.
 - Definition of “Excellent” – BES-supported research leads to important discoveries that impact the course of others’ research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries.
 - Definition of “Good” – BES-supported research leads to a steady stream of outputs of high quality.
 - Definition of “Fair” – BES-supported research leads to modest outputs of good quality.
 - Definition of “Poor” – BES-supported research leads to limited outputs.
 - How will progress be measured? – *Expert Review every three years will rate progress as “Excellent”, “Good”, “Fair” or “Poor”.*

- By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.
 - Definition of “Excellent” – BES-supported research leads to important discoveries that impact the course of others’ research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries.
 - Definition of “Good” – BES-supported research leads to a steady stream of outputs of high quality.
 - Definition of “Fair” – BES-supported research leads to modest outputs of good quality.
 - Definition of “Poor” – BES-supported research leads to limited outputs.
 - How will progress be measured? – *Expert Review every three years will rate progress as “Excellent”, “Good”, “Fair” or “Poor”.*

- By 2015, develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.
 - Definition of “Excellent” - BES-supported research leads to important discoveries that are rapidly and readily available and feed, as appropriate, into use or projected use by the Department’s technology offices, by other federal agencies, and/or by the private sector. There is evidence of substantive interactions with the Department’s technology offices in most BES program areas.
 - Definition of “Good” - BES-supported research leads to a steady stream of outputs of high quality that show the potential to impact energy research.

- Definition of “Fair” – BES-supported research leads to modest outputs of good quality that show the potential to impact energy research.
 - Definition of “Poor” – BES-supported research leads to limited outputs that show the potential to impact energy research.
 - How will progress be measured? – *Expert Review every three years will rate progress as “Excellent”, “Good”, “Fair” or “Poor”.*
- By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.
 - Definition of “Excellent” - BES-supported research leads to new concepts and designs for next-generation instruments and detectors for x-ray, neutron, and electron-beam scattering.
 - Definition of “Good” - BES-supported research leads to new instruments that are world class.
 - Definition of “Fair” – BES-supported research leads to modest outputs of good quality that show the potential to impact the concepts and designs for next generation instrumentations.
 - Definition of “Poor” – BES-supported research leads to limited outputs that show the potential to impact the concepts and designs for next generation instrumentations.
 - How will progress be measured? – *Expert Review every three years will rate progress as “Excellent”, “Good”, “Fair” or “Poor”.*



**Report of the Committee of Visitors of the
Division of Chemical Sciences, Geosciences, and Biosciences (CGBS)
to the
Basic Energy Sciences Advisory Committee
*Review of FY 2005, 2006, and 2007***

April 23-25, 2008

***Report given by Geri Richmond (Univ. of Oregon)
July 24, 2008***

FY2008 Committee of Visitors for SC-22.1
Panel Membership, March 2008
Chemical Sciences, Geosciences, and Biosciences Division

Geri Richmond	COV Chair	University of Oregon
AMO Sciences/Gas Phase Chemical Physics		
Carl Lineberger	Panel Lead	University of Colorado
Tom Gallagher	Panelist	University of Virginia
Anthony Johnson	Panelist	University of Maryland
Arthur Suits	Panelist	Wayne State University
Sotiris Xantheas	Panelist	Pacific Northwest Nat Lab
Photochemistry/Condensed Phase Chemical Physics		
Peter Rossky	Panel Lead	University of Texas
Luis Echegoyen	Panelist	NSF/Clemson University
Etsuko Fujita	Panelist	Brookhaven Nat Lab
Devens Gust	Panelist	Arizona State University
Sharon Hammes-Schiffer	Panelist	Penn State
Thom Orlando	Panelist	Georgia Tech
Catalysis		
Bruce Gates	Panel Lead	University of California, Davis
Cynthia Friend	Panelist	Harvard University
Horia Metiu	Panelist	University of Cal., Santa Barbara
Umit Ozkan	Panelist	Ohio State University
Simon Bare	Panelist	UOP, LLC
D. Michael Heinekey	Panelist	University of Washington
Heavy Element Chemistry/Separations and Analyses		
Carol Burns	Panel Lead	Los Alamos National Lab
Bruce Chase	Panelist	DuPont
Sue Clark	Panelist	Washington State University
William Evans	Panelist	University of California, Irvine
Michael Heaven	Panelist	Emory University
Robert Hettich	Panelist	Oak Ridge National Lab

FY2008 Committee of Visitors for SC-22.1
Panel Membership, March 2008
Chemical Sciences, Geosciences, and Biosciences Division

Geosciences

Ed Stolper	Panel Lead	Caltech
Bob Bodnar	Panelist	Virginia Tech
Randy Cygan	Panelist	Sandia National Labs
Lars Stixrude	Panelist	University College London
Jim Tyburczy	Panelist	Arizona State

Biosciences

Elizabeth Gantt	Panel Lead	University of Maryland
Robert Blankenship	Panelist	Washington University
John Richards	Panelist	Cal Tech
John Shanklin	Panelist	Brookhaven Nat Lab
Kay Simmons	Panelist	USDA

Major Findings of the COV

- We find that across the Division of CGBS, the quality of the decision making processes and the documentation by program managers is *outstanding*, reflecting the experience and professionalism of these highly talented individuals. This performance is particularly remarkable given the lack of an adequate electronic information system and the uncertainties in the budget.
- Overall, the quality of solicitation, review, recommendation, and documentation were viewed very favorably, including the quality and quantity of reviewers, the in-depth analysis by program managers, and the documentation of the process.
- Monitoring of active projects and programs suffers seriously from the lack of a comprehensive database that collects such information as publications, presentations, awards, personnel, and progress.
- There has been an increase in the use of contractors meetings as a tracking, and intellectual cross-cutting awareness mechanism, which is enthusiastically supported.

Major Findings of the COV (cont.)

- Ambiguities about the decision making process appeared for a number of laboratory reviews. We encourage the CGBS program to direct on-site reviewers to focus on “forward looking”, proposed, science rather than past accomplishments.
- Overall, the science supported in CGBS consistently reflects a high degree of intellectual depth and scientific breadth, and funded scientists are highly regarded both nationally and internationally.
- Evidence for evolution of the portfolio with respect to new investigators, and diversity among investigators is substantially anecdotal due to the lack of an electronic information system that can gather the required information.
- Significant progress has been made in several other areas, including:
Improvement in proposal solicitation, re-evaluation and refocusing of the Energy Biosciences program, an encouraging addition of highly qualified program managers and 3 new program manager positions, and a systematic program prioritization. We are encouraged by the addition of new staff positions in the Division and see this as an essential component of the new structure and priorities of the Division.

THE Recommendation of the COV

The COV recommends, *in the strongest terms*, the rigorous collection of data on all aspects of:

- Proposal solicitation
- Review
- Funding recommendation
- Proposal action
- Metrics associated with progress

Including full information on

Reviewers: Institution, BES funding status, frequency of use, performance metrics,...

PI's: Institution, funding profile, annual reports/ contractors meeting abstracts, sponsored publications, patents, presentations, awards, collaborations, project personnel, success stories, ...

***Allowing efficient management of the funding process
and
tracking of progress.***

The COV believes that an implementation timeline of three years is appropriate.

In parallel,

The COV strongly encourages:

- **The collection, *through a similar database*, of the demographics of reviewers and of those funded and declined, in a manner that is consistent with federal law.**
- **The enhancement of the representation of *women* and *underrepresented minorities* and the continued enhancement in the number of *new young investigators* in project portfolios.**

This recommendation parallels repeated calls for similar action, including:

- ***From the 2007 COV Report of the Office of High Energy Physics:***

“We recommend that documentation and access to program data continues to be improved and that data is put into electronic form ...”

- ***From the 2007 COV Report of the Office of Nuclear Physics:***

“We recommend a more extensive database of the information contained in the university grants, to facilitate tracking of the overall health of the program.”

- ***From the 2007 COV Report of the Climate Change Research Division of BER:***

“This COV is making recommendations that require additional staff and support, including the development of more complete project dossiers and the development or acquisition of electronic document management and database systems ...”

- ***From the 2005 COV Report of the CGBS of BES:***

“COV strongly recommends the development of standardized database software and a coherent BES-wide computer database ...”

- ***From the 2003 COV Report of the Department of Material Science and Engineering of BES:***

“The Office of Science information management system is **ineffective** in many ways. ...Such a database is essential for the program managers to perform their jobs.”

- ***From the 2004 COV of the Environmental Remediation Sciences Division of BER:***

“The COV believes it would be very useful if the research programs supported by BER were to set goals for, and keep records of, funding demographics in terms of underrepresented groups, junior scientists, and new investigators ...”

Finally-

Thanks to Eric Rohlfing (Acting Director of BES), John Miller (Acting Direction of CGBS), Linda Blevins (Office of Science) and all program managers, staff and associated personnel (especially Diane Marceau) for assembling review materials, being available for questions and all organizational aspects of the COV review.