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SEP 23 2014

Dr. Patricia M. Dehmer  
Acting Director  
Office of Science  
U.S. Department of Energy  
1000 Independence Avenue  
Washington, D.C. 20585

Dear Dr. Dehmer:

On behalf of the Basic Energy Sciences Advisory Committee (BESAC), I am forwarding to you the report of the 2014 Committee of Visitors (COV) for the Chemical Sciences, Geosciences, and Biosciences Division. The COV met for three days in April-May 2014 to address the standing charge to BESAC to review annually one of three BES Divisions on a rotating basis. Dr. Sharon Hammes-Schiffer of the University of Illinois at Urbana-Champaign chaired this committee.

The main new recommendation from the COV is that BES execute a strategic planning session at the division level to evaluate current directions and identify new opportunities and synergies, thereby facilitating collaboration among the programs and cooperative development of the portfolios.

The recommendations of the COV and the contents of this report were unanimously accepted and endorsed by the members of BESAC at our July 2014 meeting.

I would like to thank you for the opportunity to involve BESAC in this very important review process.

Sincerely,

A handwritten signature in blue ink that reads "John C. Hemminger".

John C. Hemminger  
Chair  
Basic Energy Sciences Advisory Committee

Enclosure

cc: Sharon Hammes-Schiffer, University of Illinois at Urbana-Champaign  
Patricia Dehmer, SC-2  
Harriet Kung, SC-22  
Katie Perine, SC-22

**Report of the Committee of Visitors  
Division of Chemical Sciences, Geosciences and Biosciences  
of the  
Basic Energy Sciences  
U.S. Department of Energy to  
the  
Basic Energy Sciences Advisory Committee**

**Review of FY 2011, 2012 and 2013**

**Germantown, Maryland  
April 30 – May 2, 2014**

## Executive Summary

A Committee of Visitors (COV), under the guidance of the Basic Energy Sciences Advisory Committee (BESAC), reviewed the programs in the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the Office of Basic Energy Sciences (BES) covering the fiscal years 2011, 2012, and 2013. Sixteen participants plus the chair met at the Germantown headquarters of BES on April 30 – May 2, 2014. The charge given to the COV by John Hemminger, Chair of the Basic Energy Sciences Advisory Committee (BESAC) was to: (i) assess the efficacy and quality of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs, (ii) within the boundaries defined by the DOE missions and available funding, comment on how the award process has affected the breadth and depth of portfolio elements, and the national and international standing of the portfolio elements. The COV was chaired by Dr. Sharon Hammes-Schiffer. The format was similar to those of previous COV reviews of programs in the Office of Science reviewing the three programmatic teams within the CSGB Division: Fundamental Interactions, Photochemistry and Biochemistry, and Chemical Transformations. The review excluded work performed in Energy Frontier Research Centers (EFRCs), the Fuels from Sunlight Energy Innovation Hub, and the Office of Science Early Career Program.

The COV judged the processes of solicitation, review, documentation, and monitoring of proposals to be outstanding, in large part due to the dedication and professionalism of the Program Managers and support staff. Moreover, the breadth and depth of the portfolio elements, as well as the quality of the science and principal investigators, were found to be excellent. The Program Managers have successfully balanced the mission-oriented nature of the DOE with the flexibility required for high-quality scientific research. The COV congratulates BES and the Office of Science on its accomplishments. This Committee appreciates the careful planning and efficiency of the Division management and staff in preparing for the review, as well as their help and responsiveness to all requests during the review.

The COV has four major recommendations:

- The COV strongly recommends a substantial increase in the funding for Program Officers to travel to national and international conferences, as well as visit the laboratories of researchers in their programs, to broaden participation in the BES programs and ensure that the research remains at the forefront of the fields.
- The COV recommends the continued use of encouraging preliminary statements of potential research projects as a mechanism for Program Managers to provide rapid feedback to potential principal investigators prior to the submission of full proposals.
- The COV recommends that the full implementation of the Portfolio Analysis and Management System be completed as soon as possible to allow analysis of data related to the reviewing process and demographics of the BES programs.
- The COV recommends that BES execute a strategic planning session at the division level to evaluate current directions and identify new opportunities and synergies, thereby facilitating collaboration among the programs and cooperative development of the portfolios.

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## 1. Introduction

This report documents the findings from a Committee of Visitors (COV) that was assembled under the auspices of the Basic Energy Sciences Advisory Committee (BESAC) to evaluate the processes and programs of the Division of Chemical Sciences, Geosciences, and Biosciences in the Office of Basic Energy Sciences (BES). The COV met at the Department of Energy facilities in Germantown, Maryland, for two and one-half days from April 30 – May 2, 2014. This was the fifth in the series of COV reviews of the CSGB Division; the first was held in January 2002, with subsequent reviews in 2005, 2008, and 2011.

## 2. The Charge to the Committee of Visitors

The charge to the COV was established in a letter from the Chair of BESAC to Dr. Sharon Hammes-Schiffer, who had agreed to chair the COV. The letter is attached as [Appendix I](#). The charge was to address the operations of the CSGB Division during fiscal years 2011, 2012, and 2013. The components of the Division to review were:

- Atomic, Molecular, and Optical Sciences
- Gas Phase Chemical Physics
- Condensed Phase and Interfacial Molecular Science
- Computational and Theoretical Chemistry
- Catalysis Science
- Separations and Analyses
- Heavy Element Chemistry
- Geosciences Research
- Solar Photochemistry
- Photosynthetic Systems
- Physical Biosciences

The committee was not charged to consider activities such as the Energy Frontier Research Centers (EFRCs), the Fuels from Sunlight Energy Innovation Hub, or the Office of Science Early Career Program.

The COV was asked to evaluate the following major elements: (i) For both DOE laboratory projects and grants programs, assess the efficacy and quality of the process used to solicit, review, recommend, and document proposal actions and to monitor active projects and programs; (ii) Within the boundaries defined by the DOE missions and available funding, comment on how the award process has affected the breadth and depth of portfolio elements, and the national and international standing of the portfolio elements.

## 3. The Committee Membership

The COV membership was selected by the COV chair, Dr. Sharon Hammes-Schiffer, in consultation with BES staff to represent a cross-section of experts in scientific fields relevant to the activities supported by the CSGB Division. A balance was achieved between researchers who currently receive funding from BES and those who do not (10 and 7, respectively),

between academic (12), national laboratory (4) and industrial (1) researchers, between those who have previously served on the CSGB COV and those who have not (4 and 13, respectively). In addition, Dr. Joseph Francisco from Purdue University was slated to be a member of the COV but was unable to attend at the last minute due to personal reasons.

A full listing of the COV members and their panel assignments for both the first and second reading of the folders is given in [Appendix II](#) and [Appendix III](#), respectively. The COV consisted of a total of 16 members, plus the chair, divided among 3 panels. For each panel a Lead was selected, who was responsible for leading the panel to produce a written summary of findings, comments, recommendations, and ratings of progress toward achieving long-range BES goals. The programs were divided as follows:

Panel 1: Fundamental Interactions – Panel Lead: Bruce Kay  
Atomic, Molecular, and Optical Sciences  
Gas Phase Chemical Physics  
Condensed Phase and Interfacial Molecular Science  
Computational and Theoretical Chemistry

Panel 2: Photochemistry and Biochemistry – Panel Lead: Jim McCusker  
Solar Photochemistry  
Photosynthetic Systems  
Physical Biosciences

Panel 3: Chemical Transformations – Panel Lead: Nick Winograd  
Catalysis Science  
Separations and Analysis  
Heavy Element Chemistry  
Geosciences

## 4. The Review Process

The COV assembled in Germantown at 8:30 AM on Wednesday, April 30, and adjourned at 2:00 PM on Friday, May 2. The agenda for the COV is attached as [Appendix IV](#).

Prior to convening in Germantown, each COV member was supplied with the link to the CSGB COV website containing a comprehensive set of information pertaining to: the COV process, the report template, the core research activities of the Division, the procedures used by BES in reviewing both university and national laboratory applications, and a copy of the 2011 CSGB Division COV report together with the response from BES. This information was extremely useful and easy to access through the COV website. In addition, the COV members participated in a conference call approximately one month prior to the review, and the chair and panel leads participated in a conference call approximately one week prior to the review. Several BES staff also participated in these conference calls, which were initiated by John Miller. The first conference call was helpful in terms of providing information to the panel members and answering their questions, and the second conference was useful in terms of

finalizing the procedural details of the review. Additional information was also supplied to each member during the COV review in Germantown, including copies of the plenary presentations and a more detailed overview of each of the Division's programs.

The COV began with a reiteration of the charge to the committee given by the BESAC chair, Prof. John Hemminger. Dr. Harriet Kung, Director of BES, presented an overview of BES followed by an overview of the CSGB Division by Dr. Michael Casassa, Acting Director of CSGB. Dr. Jeff Krause presented information on the new Portfolio Analysis and Management System (PAMS) system, and Dr. John Miller briefed the committee on review procedures. The panel members were then presented with further details of the overall review process and schedule by the COV Chair, Dr. Sharon Hammes-Schiffer, before adjourning to their panel break-out rooms.

The first reading of the folders began with an overview of the Team programs by the CSGB Division Team Lead and the respective program managers. Each panel was supplied with a set of proposal folders to evaluate the CSGB Division award/decline/monitor process. These proposals were distributed among four types of programmatic decisions: easy awards, easy declines, difficult awards, and difficult declines, with 4 – 6 proposals in each program area for a total about 30 proposals per panel. The projects included laboratory-based field work proposals (FWPs) and university grants.

The panels were free to request any additional information that they felt would help them in their evaluation process. After the initial discussion period, the program managers were not present during the review process but were on hand to answer questions or provide additional input as needed.

The first reading of the files occupied the remainder of the first day, providing a thorough examination of the programs most closely related to the expertise of the participating COV panelists. Each panel prepared preliminary conclusions that were discussed with the COV chair and shared with BES senior management. The checklist used by the panels during their review of the files is presented in [Appendix V](#); it correlates with the report templates used by the panels as presented in [Appendix VI](#).

On the afternoon of the second day, the panel members were assigned to different panels outside their primary expertise for the second read. The panel leads, however, did not rotate to preserve continuity and context for the second read members. The second read allowed for further refinement of issues considered important in the preliminary findings of the first read.

At the end of the afternoon of the second day, the original members of each panel reconvened with the panel lead to merge and finalize the findings from the first and second reads, and to prepare materials for the final report. The entire COV then met in executive session to discuss and reach consensus on the major findings and recommendations.

On the third day the COV Chair and panel leads met and presented the major findings and recommendations to BES leadership, CSGB Division management, and the CSGB Division program managers.



The written reports from the panels ([Appendix VII](#)) and the conclusions and recommendations drawn from the executive session provided the basis for this report.

## **5. Major Findings of the COV**

1. The COV finds the processes of solicitation, review, documentation, and monitoring of proposals to be outstanding. The reviewing process is comprehensive and thoughtful, and the use of both mail reviews and panel reviews is viewed favorably. The Program Managers are to be commended for their dedication, professionalism, and effectiveness.
2. The COV judges the breadth and depth of the portfolio elements, as well as the quality of the science and principal investigators, to be excellent. The Program Managers have successfully balanced the mission-oriented nature of the DOE with the flexibility required for high-quality scientific research. The portfolios include many senior scientists who are highly respected at the international level, as well as more junior scientists with promising career trajectories.
3. The practice of encouraging preliminary statements of potential research projects, that is, white papers, with feedback by the Program Managers is viewed favorably. This practice allows helpful, rapid communication between the Program Manager and the potential principal investigator prior to submission of a full proposal. Such feedback discourages scientists from spending time preparing proposals that are not within the programmatic scope and provides guidance as to how scientists can refine their proposals to be more suitable for the BES mission.
4. The COV is pleased that the PAMS has been initiated, although the full implementation is not yet complete. The full implementation will provide useful quantitative information about demographics and review procedures.

## **6. Major Recommendations of the COV**

1. The COV strongly recommends a substantial increase in the funding provided to Program Officers to travel to national and international conferences, as well as to visit the laboratories of researchers in their programs. Attending conferences will enable the Program Managers to identify cutting-edge areas of research and promising researchers and to transmit the BES program message to a broader audience. Visiting the laboratories of principal investigators will allow the Program Managers to maintain closer contact with these researchers and to discuss new research directions within their programs. Overall, increased travel is expected to broaden participation in the BES programs and ensure that the research remains at the forefront of the fields.
2. The COV recommends the continued use of white papers as a mechanism for Program Managers to interact with potential principal investigators prior to the submission of proposals. This practice allows Program Managers to encourage researchers to submit a full proposal, to modify their research directions to be in accordance with programmatic considerations, or to consider alternative funding options if the topic is



not aligned with the BES mission.

3. Although the development of the PAMS is viewed favorably, the COV recommends that the full implementation of this system be completed as soon as possible to allow analysis of data that are directly relevant to the BES programs. Such data will be critical for determining how the reviewing process could be improved and in which directions participation could be broadened.
4. The COV recommends that BES execute a strategic planning session at the division level to evaluate current directions and identify new opportunities and synergies. This type of strategic planning will facilitate communication and collaboration among the programs and will encourage the Program Managers to develop their portfolios in a consistent and cooperative manner. A clarification of the objectives and vision of the CSGB Division, as well as the individual programs, will also be helpful to potential principal investigators submitting proposals. Strategic planning should be an ongoing exercise at both the team level and the division level and should involve input from the community and principal investigators as well as guidance from external sources such as BESAC reports.

## **7. Other Comments and Suggestions of the COV**

- For site reviews of proposals from national laboratories, the reviewers are given clear instructions about the review criteria, but this is not always the case for mail reviews of these proposals. The COV suggests that the mail reviewers be sent clear instructions about the review criteria, such as the emphasis on synergy, for these types of proposals.
- The balance of funding between proposals with a single principal investigator and those with multiple principal investigators is of interest to the community. A comparison of the productivity from these two types of grants would be helpful in the evaluation of this balance, although the quantification of productivity and the measurement of synergy in multiple principal investigator grants is challenging.
- While the practice of using white papers is highly commended, this practice leads to higher apparent acceptance rates because some proposals are discouraged prior to submission. The documentation of when white papers are used would provide more relevant statistics about acceptance rates. The COV recognizes that the documentation of the details of the white paper process would be burdensome and does not consider such detailed documentation to be necessary.
- The COV encourages further documentation of collaborations and interactions between programs. This documentation would enable BES to highlight this positive aspect.

# Appendix I: Charge from the Chair of BESAC, Prof. John Hemminger to the Chair of the COV, Dr. Sharon Hammes-Schiffer.

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October 7, 2013

Professor Sharon Hammes-Schiffer  
Swanlund Professor of Chemistry  
A410 CLSL  
Department of Chemistry  
University of Illinois  
600 South Mathews Avenue  
Urbana, IL 61801

Dear Professor Hammes-Schiffer:

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 2011, 2012, and 2013. 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 Research
- (3) Catalysis Science
- (4) Separations and Analyses
- (5) Heavy Element Chemistry
- (6) Geosciences Research
- (7) Solar Photochemistry
- (8) Photosynthetic Systems
- (9) Physical Biosciences

You will be provided with background material on these program elements prior to the meeting. The COV is scheduled to take place in April 30 – May 2, 2014 at the BES/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A presentation to BESAC is requested at its Summer 2014 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.

If you have any questions regarding BESAC or its legalities, please contact Katie Perine, Office of Basic Energy Sciences at 301-903-6529 or by e-mail at [katie.perine@science.doe.gov](mailto:katie.perine@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](mailto:diane.marceau@science.doe.gov). For questions related to the Chemical Sciences, Geosciences, and Biosciences Division, please contact Acting Director John Miller, 301-903-5806, or by e-mail at [john.miller@science.doe.gov](mailto:john.miller@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](mailto:jchemmin@uci.edu).

Sincerely,



Digitally signed by John  
Hemminger  
DN: cn=John Hemminger,  
o=University of California, Irvine,  
ou=Office of Research,  
email=jchemmin@uci.edu, c=US  
Date: 2013.10.06 21:22:38 -0700

John C. Hemminger, Chair  
Basic Energy Sciences Advisory Committee

Attachment

cc: H. Kung  
J. Miller  
K. Perine  
D. Marceau

## Appendix II: COV Members and Contact Information

Last Name	First Name	Institution	Email
Boncella	James	LANL	<a href="mailto:boncella@lanl.gov">boncella@lanl.gov</a>
Broderick	Joan	Montana State U	<a href="mailto:jbroderick@chemistry.montana.edu">jbroderick@chemistry.montana.edu</a>
Chaka	Anne	PNNL	<a href="mailto:Anne.Chaka@pnnl.gov">Anne.Chaka@pnnl.gov</a>
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Lewandowski	Heather	JILA/CU	<a href="mailto:lewandoh@colorado.edu">lewandoh@colorado.edu</a>
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Rustad	Jim	Corning	<a href="mailto:rustadjr@corning.com">rustadjr@corning.com</a>
Scholes	Greg	U of Toronto	<a href="mailto:gscholes@chem.utoronto.ca">gscholes@chem.utoronto.ca</a>
Smith	Emily	Iowa State	<a href="mailto:esmith1@iastate.edu">esmith1@iastate.edu</a>
Turro	Claudia	Ohio State	<a href="mailto:turro@chemistry.ohio-state.edu">turro@chemistry.ohio-state.edu</a>
Utschig	Lisa	Argonne	<a href="mailto:utschig@anl.gov">utschig@anl.gov</a>
Winograd **	Nick	Penn State	<a href="mailto:nxw@psu.edu">nxw@psu.edu</a>

\* COV Chair

\*\* Panel Lead

## Appendix III: COV Panel Assignments

FY2014 Committee of Visitors

Chemical Sciences, Geosciences, and Biosciences Division

<b>First Panel Read</b>			
<b>Panel 1 - Fundamental Interactions Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	<b>Expertise</b>
<b>Bruce Kay</b>	<b>PNNL</b>	<b>Panel Chair</b>	
Heather Lewandowski	JILA/CU	Subject Matter Expert	Atomic, Molecular, and Optical Sciences
Giulia Galli	U of Chicago	Subject Matter Expert	Chemical Physics - Gas Phase
Gilbert Nathanson	Wisconsin	Subject Matter Expert	Chemical Physics - CPIMS
Rigoberto Hernandez	Ga. Tech	Subject Matter Expert	Chemical Physics - Computational and Theoretical
<b>Panel 2 - Photochemistry and Biochemistry Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	<b>Expertise</b>
<b>Jim McCusker</b>	<b>Michigan State</b>	<b>Panel Chair</b>	
Greg Scholes	U of Toronto	General Expert	
Claudia Turro	Ohio State	Subject Matter Expert	Solar Photochemistry
Lisa Utschig	Argonne	Subject Matter Expert	Photosynthetic Systems
Joan Broderick	Montana State U	Subject Matter Expert	Physical Biosciences
<b>Panel 3 - Chemical Transformations Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	<b>Expertise</b>
<b>Nick Winograd</b>	<b>Penn State</b>	<b>Panel Chair</b>	
Jim Rustad	Corning	Industry Expert	
Nicholas Delgass	Purdue	Subject Matter Expert	Catalysis Science
Emily Smith	Iowa State	Subject Matter Expert	Separations and Analysis
James Boncella	LANL	Subject Matter Expert	Heavy Element Chemistry
Anne Chaka	PNNL	Subject Matter Expert	Geosciences

<b>Second Panel Read</b>			
<b>Panel 1 - Fundamental Interactions Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	
<b>Bruce Kay</b>	<b>PNNL</b>	<b>Panel Chair</b>	
Nicholas Delgass	Purdue		
Emily Smith	Iowa State		
James Boncella	LANL		
Anne Chaka	PNNL		
<b>Panel 2 - Photochemistry and Biochemistry Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	
<b>Jim McCusker</b>	<b>Michigan State</b>	<b>Panel Chair</b>	
Giulia Galli	U of Chicago		
Rigoberto Hernandez	Ga Tech		
Heather Lewandowski	JILA/CU		
Gilbert Nathanson	Wisconsin		
Jim Rustad	Corning		
<b>Panel 3 - Chemical Transformations Team</b>			
<b>Name</b>	<b>Institution</b>	<b>Role</b>	
<b>Nick Winograd</b>	<b>Penn State</b>	<b>Panel Chair</b>	
Greg Scholes	U of Toronto		
Claudia Turro	Ohio State		
Lisa Utschig	Argonne		
Joan Broderick	Montana State		

<b>Panelist unable to attend:</b>	
Joe Francisco	Purdue

## Appendix IV: COV Agenda

**AGENDA**  
**Basic Energy Sciences Advisory Committee**  
**Committee of Visitors for the**  
**Chemical Sciences, Geosciences, and Biosciences Division**  
**April 30 – May 2, 2014**

Tuesday, April 29, 2014				
Time	Activity	Committee Members	Division Staff	Location
6:30 PM	Optional, Informal Reception	All		TBD

Wednesday, April 30, 2014				
Time	Activity	Committee Members	Division Staff	Location
7:30 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
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	All	Harriet Kung, Director Office of Basic Energy Sciences	A-410
9:00 AM	Overview of the Chemical Sciences, Geosciences, and Biosciences Division	All	Michael Casassa, Acting Director Chemical Sciences, Geosciences, and Biosciences Division	A-410
9:30 AM	Update on the SC Portfolio Analysis and Management System (PAMS)	All	Jeff Krause, Acting Team Lead	A-410
9:50 AM	Review Procedures	All	John Miller, Team Lead	A-410
10:15 AM	Instructions and Schedule	All	Sharon Hammes-Schiffer, Chair Committee of Visitors	A-410
10:30 AM	Break and disperse to panel rooms			
10:45 AM	<b>First Read Panel 1</b> Fundamental Interactions Team	Panel 1 Members	Jeff Krause, Acting Team Lead Greg Fiechtner, Wade Sisk, Tom Settersten (detailee), Mark Pederson	E-401
10:45 AM	<b>First Read Panel 2</b> Photochemistry and Biochemistry Team	Panel 2 Members	Gail McLean, Team Lead Chris Fecko, Mark Spitler, Bob Stack, Nada Dimitrijevic (detailee)	G-426

10:45 AM	<b>First Read Panel 3</b> Chemical Transformations Team	Panel 3 Members	John Miller, Team Lead Raul Miranda, Paul Maupin, Larry Rahn, Philip Wilk, Nick Woodward	E-301
12:30 PM	Lunch	All	All	A-410
1:30 PM	<b>Resume First Read Panels</b>	Panels		Panel Rooms
4:00 PM	Preliminary Report Drafting – Key Elements and Gaps	Panels		Panel Rooms
5:00 PM	Meeting between Panel Leads and Chair	Panel Leads and Chair		F-441
5:30 PM	Meeting with Chair and BES Senior Management	Chair	Harriet Kung, Michael Casassa	F-405
5:45 PM	Return to Hotel	All	Drivers with cars or walk	A-410
6:30 PM	Pickup at hotel for transport to dinner	All	Drivers with cars	Fairfield Inn Lobby
7:00 PM	Dinner for COV and BES Staff	All	All	That's Amore

<b>Thursday, May 1, 2014</b>				
<b>Time</b>	<b>Activity</b>	<b>Committee Members</b>	<b>Division Staff</b>	<b>Location</b>
7:45 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
8:30 AM	Fundamental Interactions Team Session	Panel 1	Jeff Krause, Acting Team Lead Greg Fiechtner, Wade Sisk, Tom Settersten (detailee), Mark Pederson	E-401
8:30 AM	Photo- and Biochemistry Team Session	Panel 2	Gail McLean, Team Lead Chris Fecko, Mark Spitler, Bob Stack, Nada Dimitrijevic (detailee)	G-426
8:30 AM	Chemical Transformations Team Session	Panel 3	John Miller, Team Lead Raul Miranda, Paul Maupin, Larry Rahn, Philip Wilk, Nick Woodward	E-301
9:15 AM	<b>Complete First Read Panel Reports</b>	Panels		Panel Rooms



11:15 AM	COV Executive Session Reports from Panel Leads on First Read Reports	All		A-410
12:30 PM	<b>Lunch</b>	<b>All</b>		A-410
1:30 PM	<b>Second Read Panel 1</b> Fundamental Interactions Team	Panel 1 Second Read Members	Jeff Krause, Acting Team Lead Greg Fiechtner, Wade Sisk, Tom Settersten (detailee), Mark Pederson	E-401
1:30 PM	<b>Second Read Panel 2</b> Photochemistry and Biochemistry	Panel 2 Second Read Members	Gail McLean, Team Lead Chris Fecko, Mark Spitler, Nada Dimitrijevic (detailee), Bob Stack	G-426
1:30 PM	<b>Second Read Panel 3</b> Chemical Transformations	Panel 3 Second Read Members	John Miller, Team Lead Raul Miranda, Paul Maupin, Larry Rahn, Philip Wilk, Nick Woodward	E-301
3:30 PM	Merge First and Second Read Input Finalize Draft Panel Reports	First Read Panels		Panel Rooms
4:00 PM	COV Executive Session	All		A-410
5:30 PM	Return to hotel	All	Drivers with cars or walk	A-410
	Dinner on your own	All	None	Local restaurant information provided

<b>Friday, May 2, 2014</b>				
<b>Time</b>	<b>Activity</b>	<b>Committee Members</b>	<b>Division Staff</b>	<b>Location</b>
7:45 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
8:30 AM	Closeout Session with COV and BES Senior Management and Staff	All		A-410
10:00 AM	Leave for airport from Germantown	All		

## Appendix V: Checklists for COV review

Checklist for COV Review -- CSGB Grant Award Process	
	Comments
<b>I. Efficacy and Quality of Processes</b>	
(a) Solicit, review, recommend and document proposal actions	
(b) Monitor active projects and programs	
<b>Review Process:</b> Consider, for example:	
Sufficient number of reviews?	
Qualified reviewers?	
Quality of reviews (consistent with criteria)?	
<b>Documentation and Monitoring:</b> Consider, for example:	
Completeness of selection statement?	
Revised budgets?	
Content of declination summary?	
Continuation/Annual reports?	
<b>II. Impact and Standing of Portfolio Elements</b>	
(a) Award breadth and quality: Consider, for example:	
Potential and/or actual impact evident?	
Balance of innovation and risk?	
Technical diversity?	
Complement the CRA's research portfolio?	
Relevant to the DOE's mission?	
Size and duration of award?	
<b>III. Impact and Standing of Portfolio Elements</b>	
(b) National and International Standing. Consider, for example:	
PIs national/international leaders in their fields?	

Checklist for COV Review -- CSGB National Laboratory Award Process	
	Comments
<b>I. Efficacy and Quality of Processes</b>	
(a) Solicit, review, recommend and document proposal actions	
(b) Monitor active projects and programs	
<b>Review Process:</b> Consider, for example:	
Sufficient number of reviews?	
Qualified reviewers?	
Quality of reviews (consistent with criteria)?	
Adequacy of on-site review process?	
<b>Documentation and Monitoring:</b> Consider, for example:	
Completeness of review summary?	
Appropriateness/clarity of Guidance Letter and Action Items?	
Adequacy of laboratory response to Action Items (if appropriate)?	
Synergistic effort appropriate for National Laboratory program?	
<b>II. Impact and Standing of Portfolio Elements</b>	
(a) Award breadth and quality: Consider, for example:	
Potential and/or actual impact evident?	
Balance of innovation and risk?	
Technical diversity?	
Complement the CRA's research portfolio?	
Relevant to the DOE's mission?	
Size and duration of award?	
<b>III. Impact and Standing of Portfolio Elements</b>	
(b) National and International Standing. Consider, for example:	
PIs national/international leaders in their fields?	

# Appendix VI: First Read/Second Read COV Report Template

## PANEL REPORT TEMPLATE

### BES COMMITTEE OF VISITORS (COV)

Reviewing the Chemical Sciences, Geosciences and Biosciences Division

#### **Based on the Charge to the COV:**

1) For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:

- (a) solicit, review, recommend, and document proposal actions and
- (b) monitor active project and programs.

(2) Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:

- (a) the breadth and depth of portfolio elements, and
- (b) the national and international standing of the portfolio elements.

#### **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**

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
- PI 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
- 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 progress and impact
- the stature of the principal investigators in their fields
- the leadership position in the nation and the world

Findings:

Comments:

Recommendations:

## **Appendix VII: Summary Reports from the Three Panels**

- Panel 1. Fundamental Interactions
- Panel 2. Photochemistry and Biochemistry
- Panel 3. Chemical Transformations

**Panel 1. FUNDAMENTAL INTERACTIONS**  
BES COMMITTEE OF VISITORS (COV)  
Reviewing the Chemical Sciences, Geosciences and Biosciences Division

**Based on the Charge to the COV:**

- 1) For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
  - (a) solicit, review, recommend, and document proposal actions and
  - (b) monitor active project and programs.
  
- (2) Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
  - (a) the breadth and depth of portfolio elements, and
  - (b) the national and international standing of the portfolio elements.

**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**

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:

The Fundamental Interactions Team of CSGB is comprised of four core programs: Atomic, Molecular, and Optical Sciences (AMOS), Gas-Phase Chemical Physics (GPCP), Condensed Phase and Interfacial Molecular Sciences (CPIMS), and Computational and Theoretical Chemistry (CTC). All four of these have strong representation in both Universities and National Laboratories.

Program Managers in all four core programs are doing an outstanding job assessing proposals and making funding decisions. Each of the proposals surveyed had a reasonable number (4-6) of reviewers who made reasoned comments. The reviewers were chosen primarily based on scientific expertise but appeared to represent diversity in other areas such as seniority and gender. The Program Managers correctly and appropriately contextualized reviewer's assessments within the framework of the PI's past results, the PI's funding portfolio, and previous grant reviews, as well as the fit to the core program.

They are commended for including detailed, compelling, and clear arguments for their funding decisions in their selection statements. The Program Managers also appreciate the importance of communicating the reasons for current actions and providing advice on future proposal submission, and in many cases this advice was provided in follow-on phone conversations with the PI. Both the first- and second-read panels commented positively on the depth, detail, and thoroughness of the funding decision reports provided by the Program Managers.

Program Managers employ varying strategies to solicit the submission of new proposals, including direct informal discussions, phone calls, and white papers. This flexibility is viewed as positive but makes it difficult to track actual success statistics.

Comments:

It is an unfortunate fact that budgets are tight. As such, Program Managers have little choice but to factor costs in some way. Nevertheless, it appears that choices are ultimately based on the relative scientific merits and thematic fit to the program rather than proposal budget.

The panel was impressed by the method in which proposals that were not selected for renewal were terminated. The so-called “Terminal Renewal” provides the PI with a limited amount of follow-on funding (typically one year’s support) to wind down their research effort. This facilitates “soft landing” students and postdocs, and documenting the accomplished research in publications.

The panel is excited about the incoming use of PAMS as a way to track proposals, white papers, and other queries for new research directions.

Recommendations:

We recommend implementation and deployment of the PAMS data tracking system and look forward to the statistical data it will be able to generate through database mining.

**(b) Monitor active project and programs**

Consider, for example

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

Findings:

Progress reports were well written by PIs and well integrated by Program Managers in the files used to track proposals. It was not clear from the files how the progress reports were used by the Program Managers, but discussions with them indicated that these reports were used to monitor progress through tracking publications and spending rates.



PI meetings remain a critical component for maintaining and advancing the mission focus within the core program portfolios. These meetings provide a forum for the PIs to interact with each other and the Program Managers on an annual basis and can serve as a catalyst for generating new ideas and research partnerships between various PIs and institutions.

On-site reviews and visits of National Laboratory and multi-investigator programs were performed at the same high level as single-investigator mail reviews. These on-site reviews are especially important for the National Laboratory programs, as they provide a means for the reviewers to evaluate the synergistic team nature and DOE mission relevance of these typically large and multi-investigator programs.

Comments:

We strongly encourage that Program Managers increase their attendance at national scientific meetings. These visits would increase their visibility and interactions with the scientific community. Specifically, Program Managers could learn about potential new scientific directions, identify new potential investigators, and educate the community about the BES portfolio and mission. Either the travel budget needs to be increased or alternate mechanisms (perhaps through virtual attendance or Webinars) should be considered and implemented to achieve these goals.

Recommendations:

We recommend that travel budgets for Program Managers be increased so they can attend national scientific meetings and topical conferences relevant to their 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**

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
- the appropriateness of award scope, size, and duration

Findings:

The overall quality of the scientific programs at both Universities and National

Laboratories is exceptional. The balance of projects between risk, innovation, and mission relevance has been excellent up to now, but is being challenged by the limited number of new starts available in the current funding climate.

Program Managers are maintaining continuity in their programs both through managing individual investigators and their related research thrusts. Through direct discussions with the four Program Managers, the panel found that they were extraordinarily insightful and enthusiastic about broadening their portfolios through the addition of new investigators and new research directions. The panel commends the Program Managers for their dedication and optimism. Regrettably, these laudable goals prove difficult to implement in times of flat or decreasing program budgets.

The portfolio in Fundamental Interactions is well aligned (including co-funded grants) with other parts of the Division. Additionally, each of the three core programs that have experimental elements make effective use of the resources (nanocenters, neutron sources, and light sources) provided by the Scientific User Facilities Division (SUF) of BES. Many of the projects having theoretical and computational components benefit greatly from the National Energy Research Scientific Computing Center (NERSC).

The panel was impressed by the care and thoughtfulness of the Program Managers in optimizing the size and duration of the awards relative to the scope and complexity of the research task. Such balancing is crucial for ensuring the success of the individual programs and the overall portfolio.

The role of the Program Managers in portfolio management and long-range planning is critical to the success and longevity of the programs. It appears that each core program is being managed effectively. However, it is generally unclear how these activities are being coordinated between different core programs within Fundamental Interactions and among the three teams in CSGB. Notable exceptions include the strong integration of computational and theoretical chemistry (CTC) into the Chemical Physics (GPCP and CPIMS) and AMOS core programs.

#### Comments:

There has been a lot of attention given to the funding of new young investigators and their retention in the programs, however there is less attention to new starts outside the existing investigator pool otherwise. For example, some core programs have funded few or no new grants to non-continuing PIs in the past year or two due to severe funding constraints. The existence of a comparatively low number of new starts for these potential new investigators should be addressed in some way.

#### Recommendations:

We recommend the development and deployment of a strategic planning process to better coordinate research priorities between the core programs and with other CSGB teams and BES divisions.

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

Consider, for example:

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

Findings:

In all four core programs, important and impactful research is being carried out at both Universities and National Laboratories. This work is at the forefront of international energy research, and many of the PIs are world-renowned authorities in their fields, or on a trajectory toward becoming such leaders. This is evidenced by the number of publications in prestigious journals, the frequency of plenary and invited talks at national and international conferences, and the number of awards, prizes, fellowships, and academy memberships.

Comments:

While BES can and should be extremely proud of the leadership position it has achieved in Chemical Physics and Atomic, Molecular, and Optical Science, it is important to realize that maintaining this position in an increasingly competitive world will require significant funding increases in the near future.

Recommendations: None

## **Panel 2. PHOTOCHEMISTRY AND BIOCHEMISTRY**

BES COMMITTEE OF VISITORS (COV)

Reviewing the Chemical Sciences, Geosciences and Biosciences Division

### **Based on the Charge to the COV:**

1) For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:

- (a) solicit, review, recommend, and document proposal actions and
- (b) monitor active project and programs.

(2) Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:

- (a) the breadth and depth of portfolio elements, and
- (b) the national and international standing of the portfolio elements.

### **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**

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:

The Photochemistry and Biochemistry portion of CSGB is comprised of three programs: Solar Photochemistry, Photosynthetic Systems, and Physical Biosciences. All three have strong representation in universities and several national laboratories.

The proposal review process was viewed to be excellent in nearly all aspects, including the number of reviews obtained, the substantive nature of the reviews, the expertise of the reviewers chosen, as well as their diversity in terms of gender balance and those who are funded by DOE-BES versus not current supported by the program. This latter point was perceived to be an excellent way to ensure an unbiased assessment of the science being selected for support as part of a given program. The decision window was typically reasonable (5-6 months), but the panel did note a rather wide range was evident (3-12 months). Funding decisions were uniformly well supported by reviewer comments and/or

portfolio considerations. Borderline decisions were particularly well handled, with declinations based on critical problems with the science, weakness in the overall proposal, or questions about relevance to the portfolio or overall program mission. In contrast, positive decisions were conferred upon borderline proposals that had certain scientific concerns but represented areas that the Program Managers felt were potentially important contributions to the program. This is reflective of a recurring theme noted by the panel, namely the deep engagement of the Program Managers in shaping their respective programs in a way that successfully strikes an important balance between mission focus and the flexibility necessary to pursue fundamental research.

The panel was particularly impressed by the attention paid to the reviews, as well as the willingness of the Program Manager to modify what would and would not be supported (even at the level of portions of a proposal) based on these comments and portfolio considerations.

Comments: None.

Recommendations: None.

**(b) Monitor active project and programs**

Consider, for example

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

Findings:

In general, the interactions between the Program Managers and the PIs for ongoing research efforts is substantial and substantive; the panel was extremely impressed with the level of engagement of the Program Officers in the research efforts of the PIs they support. Particularly effective vehicles for mission focus are the contractor's meetings, which are widely perceived as being exceptional in terms of their quality as well as being an excellent mechanism to foster synergy within and between programs. The panel noted that all programs would be enhanced even further if more extensive travel options for Program Managers (e.g., national and international meetings, on-site visits, etc.) were made possible.

With regard to the National Laboratories, the panel viewed the site visit model as an exceptionally effective mechanism for evaluating these large, complex programs. The review panels (as well as mail-in reviews when needed) were of the highest caliber in terms of their scientific expertise; the balance of the review panels was generally quite good with regard to gender as well as university versus national lab backgrounds. The reviews themselves were remarkable in terms of their thoroughness and candor, thereby providing the Program Managers and PIs alike with extremely useful insights and

suggestions. The panel was struck by the fact that each individual on a given site review panel provided reviews of all aspects of the site visits (e.g., evaluation of all subtasks). In some cases this seemed to be an excessive burden on the reviewers, but it was not clear based on the available documentation whether this was a requirement by DOE or merely a choice by each reviewer.

The panel was particularly impressed with the manner in which the Program Officers used the recommendations of the panel to constructively reshape, enhance, and/or cut research efforts as needed to strengthen the program (and, in some cases, ensure mission focus). This was again reflective of the deep level of engagement by DOE personnel in the continued success of the various programs under their watch. The guidance letters transmitted to the programs were clear and accurately reflected the content of the reviews. In return, the lab responses were generally quite reasonable and appropriately responsive to DOE's comments.

Comments:

The Program Managers place an appropriately high premium on the need for synergy in the research efforts at the labs and, in nearly all cases, the labs were as well. An important consequence of this is that the lab efforts were nearly always more than the sum of their parts. The panel viewed this as highly commendable and agreed that it should be encouraged as an important metric for evaluations in the future.

The panel did note that the time lag for the overall review process seemed rather drawn out; in some cases the time between the initial letter notifying the lab of a site visit and the final paperwork being completed was in excess of a year. This may be an unavoidable consequence of the complexity of the lab operations, but the panel felt this was an issue that deserved notation.

Recommendations:

The DOE should consider putting a statement of charge in the letter to the site reviewers of National Laboratory programs to better clarify their specific responsibilities. This could be phrased along the lines of, "Your primary responsibility will be to evaluate TEAM X as well as provide your sense of the overall synergy of the research effort. You are, of course, welcome to comment on any other aspect of the site visit as you see fit." This may have the added benefit of achieving a level of consistency for site visits across the various subdivisions within the 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**

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
- the appropriateness of award scope, size, and duration

#### Findings:

In the opinion of the panel, the overall quality of the research across all three programs was exceptional. All of the portfolios were very impressive, particularly with regard to the balance between mission focus and scientific breadth. The panel was particularly impressed with the breadth of the Solar Photochemistry program, which appears to have broadened in a very positive manner over the last several years to a point where interconnections across various efforts in CSGB are clear and beginning to bear fruit in the form of jointly funded proposals and increased interdisciplinary efforts. Moreover, all of this has occurred without sacrificing the core research focus of the program. There was a clear dynamic within each program (but particularly evident in the Solar Photochemistry program) that reflected an ongoing evaluation by the Program Managers of the scientific content of the program and an effort to keep pace with the evolution of the field. The panel also noted the success associated with the recent creation of distinct programs in Photosynthetic Systems and Physical Biosciences. Of particular note is the Program Managers' success in identifying energy-relevant topics in biological systems that is allowing DOE to define a footprint in bioscience that is distinct from efforts within other agencies: this was viewed as a particularly noteworthy success that should be commended. The positive impressions just described applied equally to the university and national lab-based research efforts.

In general, the panel felt that the Program Managers are doing an excellent job with resource management given the inherent limitations associated with their budgets. The panel was particularly impressed with the willingness of Program Managers to scale back and/or terminate efforts that were deemed by them – and without exception supported by reviewers' concerns – to be drifting too far from the core focus of their program. In this regard, the Program Officers are displaying exemplary leadership in terms of actively managing their research portfolios.

#### Comments:

The panel viewed favorably the so-called “terminal” grant model, in which PIs whose projects and/or proposals were problematic were not immediately cut to zero, but rather scaled back in an effort to either allow the project to end in a reasonable fashion or as a precursor to proposal resubmission. This practice was viewed to be a remarkably effective mode of operation and a model that other federal funding agencies would do well to emulate.



The manner in which risky or “out-of-the-box” thinking is encouraged was not clear, particularly in the case of national laboratory efforts where the PIs were generally part of a larger, integrated effort. The Division may wish to consider mechanisms by which this sort of goal could be achieved.

In accord with the panel’s highly favorable view of the new physical biosciences and photosynthetic systems branches, the Division may wish to consider convening workshops similar to those done in other areas in order to create blueprints for these programs as they continue to develop and grow.

Recommendations: None

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

Consider, for example:

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

Findings:

The PIs who are being supported at universities and national labs across all three programs represent the very best in their respective areas. The panel commented specifically about the Solar Photochemistry program, which has an international reputation for excellence in the field. The presence of researchers from all three programs at a wide range of national and international conferences is a further testament to the visibility and world-class quality of the researchers being supported by CSGB.

Comments: None

Recommendations: None

**Panel 3. CHEMICAL TRANSFORMATIONS**  
BES COMMITTEE OF VISITORS (COV)  
Reviewing the Chemical Sciences, Geosciences and Biosciences Division

**Based on the Charge to the COV:**

- 1) For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
  - (a) solicit, review, recommend, and document proposal actions and
  - (b) monitor active project and programs.
  
- (2) Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
  - (a) the breadth and depth of portfolio elements, and
  - (b) the national and international standing of the portfolio elements.

**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**

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:

Chemical Transformations program solicitations and guidelines were consistent across the board. Additional guidelines for synergy and interaction were provided to reviewers for the large laboratory programs.

The panel found that each proposal received between 4 and 7 substantive reviews. In general, the depth and thoughtfulness of the comments were of the highest quality. In addition, the Program Managers selected individuals recognized by the panel as experts. The reviews of complex multi-PI proposals from the laboratories were particularly insightful and detailed.

Program Managers made timely decisions on submitted proposals. Those proposals at the margin were acted upon promptly.

In general, selection statements by the Program Managers were thorough, thoughtful and balanced. The panel felt that a vast majority of these statements expressed the nuances and the essences of the reviewer's comments. There were isolated cases, however, where negative comments were highlighted in quotations from specific reviews, but how these comments were weighed into the evaluation process was not apparent.

Comments:

Reviews in Geosciences are particularly challenging because expertise must be found in diverse areas ranging from geochemistry to electronic structure to geophysics. Within this environment, however, excellent reviewers were identified. The only cautionary note is to be sure to include an adequate sample of reviewers from outside the DOE community.

The Heavy Element group made excellent use of international reviewers, a necessary approach due to the relatively small number of investigators in the US.

In Separations and Analysis and in Catalysis there was an excellent mix of reviewers associated with the DOE and those outside of the DOE community.

In Geosciences, internal DOE recommendation memos provided excellent highlighting of how the proposed work fit into the Geosciences portfolio and how it impacted DOE priorities.

With respect to Catalysis, the panel thought that it would be useful to include a few selected reviewers from industry who appreciate basic science. In this field these reviewers could give unique insight into the fundamental ideas that are not being tackled in the commercial arena, but where deeper understanding could have industrial impact in areas such as energy efficiency that are in line with the DOE mission.

In the information packet provided to the COV, a list of reviewers utilized by BES was included. Although this list is informative, it would be useful to associate each reviewer with the specific BES area involved in the review.

Reviews of the more complex multi-PI laboratory proposals were clearly an extraordinary burden to individuals. It would be useful if the DOE could find a way to make this task a bit easier.

The Program Managers have done a commendable job of trimming underperforming projects.

Recommendations: None

**(b) Monitor active project and programs**

Consider, for example

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

Findings:

The Program Managers appeared to actively keep abreast of ongoing projects. There was a detailed record of written progress reports from the PIs.

Comments:

Panel members felt that contractor meetings are effectively used for communication among the PIs, and for elucidation of the structure of the portfolio associated with each area. These meetings also served as a vehicle for the solicitation of ideas for new directions. Although the agenda for these meetings are on-line, more details about content would be useful for the next COV.

Information regarding site visits that were not part of the review process was not provided to the COV.

Recommendations:

The panel feels strongly that interactions between Program Managers and the laboratories are very important, and recommends that funds be provided to enhance these opportunities. In addition, we found no evidence for site visits to University facilities for the smaller research programs, an oversight that should be corrected if at all possible.

**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
- the appropriateness of award scope, size, and duration

Findings:

For Chemical Transformations, the overall quality of the science is excellent. There is a good mix between single investigator programs and larger group efforts. In the smaller areas, the program managers have made strategic selections of specific areas for the research portfolio. When reviewers pointed out high risk ventures, Program Managers were often willing to take on this risk, after providing appropriate justification.

The committee read about the relationships between programs described in each of the program write-ups, but did not examine those relationships in depth. Examples include use of BES synchrotron facilities by Catalysis, Geosciences, and the Heavy Element communities, as well as coordination between the Computation and Theoretical Chemistry Program and the Chemical Transformation Division and between Photo and Biochemistry and the Catalysis program.

Comments:

In the Catalysis area, there is good evidence for introduction of young investigators through both new starts and the early career program. The panel noted that in Separations and Analysis, there were three early career funded proposals, although all are in Separations.

The panel looks forward to information about demographics and program duration from PAMS that will hopefully be provided to the scientific community.

Future COVs should be provided specific evidence for collaboration between programs so this issue can be more thoroughly vetted.

Recommendations: None

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

Consider, for example:

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

Findings:

The panel found clear evidence that each program had PIs who are clearly world leaders in their areas. The program managers in the Chemical Transformations division provided impressive documentation about the high quality and recognition of the PIs. These data include academies, awards, prizes and publications. The Division can be proud of the people that it supports.

Comments: None

Recommendations: None