

**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 2017, 2018 and 2019**

**Virtual  
September 8 – 11, 2020**

## 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 2017, 2018, and 2019.

Seventeen participants plus the chair met over Zoom meeting September 8-11, 2020. The charge given to the COV by Cynthia Friend, Co-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. Andrew G. Stack. Due to the ongoing COVID-19 pandemic, the COV was conducted remotely using online virtual conference software. Despite the online nature of the meeting, the format was similar to those of previous COV reviews of programs in the Office of Science. This review covered the three programmatic teams within the CSGB Division: Fundamental Interactions, Photochemistry and Biochemistry and Chemical Transformations. The review included research funded in the following programs: FY 2017, FY 2018, and FY 2019 Continuation of Solicitation for The Office of Science Financial Assistance Program; FY 2017, FY 2018, and FY 2019 Early Career Research Program; FY 2017 and FY 2018 Computational Chemical Sciences; FY 2018 Research at the Frontiers of X-Ray Free Electron Laser Ultrafast Chemical and Materials Sciences; FY 2017 Scientific Discovery through Advanced Computing (SciDAC); FY 2018 and FY 2019 Materials and Chemical Sciences Research For Quantum Information Science; and FY 2019 Data Science for Discovery in Chemical and Materials Sciences. The review excluded research funded in Energy Frontier Research Centers (EFRCs), and the Fuels from Sunlight Energy Innovation Hub.

Overall, the COV found the process to solicit, review, recommend and document proposal actions to be a highly informed, thoughtful and careful process whose success is driven by the Program Managers. In considering proposals, the COV found evidence of balanced considerations of likelihood of sustained highly impactful research, mission relevance, strategic planning, past productivity and reviewer expertise. The COV found that CSGB employed a variety of methods for different types of funding opportunities and this was viewed an efficient way to address varying needs for proposal and pre-proposal evaluation. There was evidence of an active role of PMs in cultivating their portfolios to maintain alignment with strategic planning directions and incorporate new elements into their programs. These efforts were viewed as a successful way to ensure innovative research and to enhance the breadth and depth of the portfolio. Overall, the COV commends the CSGB staff for their efforts to ensure that CSGB continues to fund the most competitive and innovative research nationally and internationally.

The COV makes the following specific major recommendations:

1. While the overall review process is excellent, there is an opportunity to communicate the results of proposal review and the decision-making process more fully with PIs. Specifically, while it was evident that most PMs were reaching out to the PIs of declined

proposals with offers to communicate verbally about the results, these efforts were not always documented in the Portfolio Analysis and Management System (PAMS). This made it difficult for the COV to ascertain whether this information was being communicated to PIs. The COV therefore encourages CSGB to discuss what information is appropriate to communicate to PIs about funding recommendations and how those communications should be documented in PAMS. This would serve both as a robust internal documentation assisting the ability of the COV to assess the program, and a standardization of the information communicated with PIs.

2. In discussions with DOE personnel, it was evident that there are multiple pathways that DOE uses to educate potential PIs about BES funding opportunities, mission, and program information. These include, for example, joint webinars with the National Science Foundation and invited talks by PMs at professional meetings. However, the COV felt there may be opportunities to reach a broader audience of researchers. Thus, the COV recommends that CSGB evaluate their strategy for reaching a broad range of potential PIs and educating them about research opportunities in DOE-BES and the unique mission-driven character of BES research. A suggestion that could improve the effectiveness of outreach activities is to advertise informational webinars on the CSGB web-site next to the funding opportunity announcements.
3. In order to maintain international competitiveness and a global perspective on new research relevant to their programs, we encourage continued support of travel for PMs to attend national and international scientific meetings to maintain U.S. and BES prominence in the chemical sciences, geosciences and biosciences.
4. While maintaining the depth of individual programs, it is recommended to continue to develop research across Programs and Division boundaries and/or introduce new capabilities. This could be in the form of thematic PI meetings that cross program boundaries, or formalizing the policy of smaller seed grant opportunities for high-risk, high-reward concepts. Another mechanism could be to expand the Early Career program, and to continue to use it to bring new ideas into the respective programs. The COV recognizes that this may require funding decisions above CSGB's level.

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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 in a virtual meeting, 4 days from September 8 – 11, 2020. This was the seventh in the series of COV reviews of the CSGB Division; the first held in January 2002, with subsequent reviews in 2005, 2008, 2011, 2014 and 2017.

## 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. Andrew G. Stack, 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 2017, 2018, and 2019. 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
- Separation Science
- Heavy Element Chemistry
- Geosciences
- Solar Photochemistry
- Photosynthetic Systems
- Physical Biosciences

The review was charged to consider the following activities: FY 2017, FY 2018, and FY 2019 Continuation of Solicitation for The Office of Science Financial Assistance Program; FY 2017, FY 2018, and FY 2019 Early Career Research Program; FY 2017 and FY 2018 Computational Chemical Sciences; FY 2018 Research at the Frontiers of X-Ray Free Electron Laser Ultrafast Chemical and Materials Sciences; FY 2017 Scientific Discovery through Advanced Computing (SciDAC); FY 2018 and FY 2019 Materials and Chemical Sciences Research For Quantum Information Science; and FY 2019 Data Science for Discovery in Chemical and Materials Sciences. The committee was not charged to consider activities in the Energy Frontier Research Centers (EFRCs), or the Fuels from Sunlight Energy Innovation Hub.

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. Andrew Stack, in consultation with BES staff and panel leads 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 that do not (14 and 4, respectively), between academic (10), national laboratory (7) and other federal agencies (1), and between those who have previously served on a COV and those who have not (4 and 14, respectively). Contact information for the panelists is given in Appendix II.

A full listing of the COV members and their panel assignments for the initial review of materials provided in the Portfolio Analysis and Management System (PAMS) is given in [Appendix III](#). The COV consisted of a total of 17 members, plus the chair, divided between 3 panels. For each panel a Lead was selected, who was responsible for leading the team 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: Kelly Gaffney  
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: Joan Broderick  
Solar Photochemistry  
Photosynthetic Systems  
Physical Biosciences

Panel 3: Chemical Transformations – Panel Lead: Laura Pyrak-Nolte  
Catalysis Science  
Separations Science  
Heavy Element Chemistry  
Geosciences

### 4. The Review Process

The COV assembled via Zoom at 1:00 PM on Tuesday, September 8, and adjourned at 4:00 PM on September 11. The agenda for the COV is attached as [Appendix IV](#).

Prior to convening, each COV member was supplied with the link to the COV module in PAMS. On August 27, an information session was held to guide COV members through PAMS, and ensure that all had valid login credentials, which was helpful in minimizing the amount of

time necessary to use during the COV itself for these purposes. The Reference Materials section of the COV module contained 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 proposal, copies of the plenary presentations, and a copy of the 2017 CSGB Division COV report together with the response from BES.

The COV began with a reiteration of the charge to the committee given by the BESAC co-chair, Prof. Cynthia Friend. Dr. Linda Horton, Director of BES presented an overview of BES followed by an overview of the CSGB Division by the Division Director, Dr. Bruce Garrett. Dr. Gail McLean briefed the committee on BES CSGB review procedures. The panel members were then presented with further details of the overall COV review process and schedule by the COV Chair, Dr. Andrew Stack, before adjourning to their virtual panel break-out sessions.

The reading of the folders began with an overview of the Team programs by the CSGB Division Team Lead. Each panel was supplied with a list of proposal folders to evaluate the CSGB Division award/decline/monitor process. These proposals were distributed among four types of programmatic recommendations: easy awards, easy declines, difficult awards, and difficult declines, with 6 – 8 proposals in each program area for a total about 50 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 in a break-out room to answer questions or provide additional input as needed.

The reading of the files occupied the remainder of the first day as well as much of the next two days, providing a thorough examination of the programs most closely related to the expertise of the participating COV panelists. Pre-proposal review and selection were evaluated on September 10<sup>th</sup>. 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](#).

At the end of the afternoon of the last day, the panel members reconvened with the panel lead to merge and finalize the findings and panel leads worked with the chair 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. The COV met and the chair 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. Overall, the COV found the process to solicit, review, recommend and document proposal actions to be a highly informed, thoughtful and careful process, with balanced considerations of likelihood of sustained highly impactful research, mission relevance, strategic planning, past productivity and reviewer expertise. It is overwhelmingly evident that this excellence in process is being driven by the dedication and professionalism of the PMs. The COV members were continually impressed with the level of consideration that the PMs gave to both individual proposals and the portfolio of projects in each program. The COV strongly commends the efforts of the PMs and that of CSGB personnel.
2. The active role of PMs in strategic planning regarding the breadth and depth of portfolio elements was noted and was viewed as a successful way to improve the standing of the research in the portfolio. As an example, it was clear that successful early career awards were resulting in new methods, personnel and concepts to be included into the programs. Research priorities within CSGB are well documented and available through a variety of avenues, including the BES reports, BRNs, and individual program webpages. The sustained travel budget for PMs to attend professional society meetings is critical to maintain a global perspective on their programs.
3. To review pre-proposals and proposals, CSGB utilizes a diversity of methods depending on the type of call and number of proposals. This tailoring of methods was judged to have improved the quality of both proposals and/or reviews. For example, in the pre-proposal process for some solicitations, a three program manager down-select was used in FY19 for some programs with large numbers of pre-proposals. No evidence was found that this harmed the success rate of proposals, and it is viewed as a positive since this apparently lessens the burden on reviewers and PIs. For proposal review, the use of well-managed panels was found to improve the quality of individual reviews but the COV recognizes that their efficacy might vary on a field-by-field basis or by the type of solicitation. Overall, the COV encourages the continued use of a diversity of different methods for pre-proposal and proposal review where appropriate.
4. The principal investigator meetings were found to be an efficient method to monitor active projects and programs. They also help to build a sense of scientific community in the program. The documentation of these meetings in the form of publicly-available agendas and abstracts is helpful for both currently-funded PIs and potential PIs who are unfamiliar with CSGB. PI meetings are a feature that make DOE funding unique and uniquely valuable.
5. In general, research and PIs supported by the CSGB programs represent the best that U.S. universities and national laboratories have to offer. The PIs recognize emerging trends in their fields (not just in the U.S. but globally). The CSGB research portfolio is competitive with other U.S. agencies, and clearly leads in some areas related specifically to energy (e.g. heavy element research, solar energy and geomechanics). CSGB is actively promoting new and emerging areas to expand its breadth while maintaining its depth. CSGB does an excellent job of maintaining depth through long term funding of PIs. At the same time, CSGB is increasing its breadth through the aggressive approach taken on strategic planning

and cross program-cutting themes. For example, CSGB's incorporation of data science into the program is impressive and has led to significant scientific impact well beyond CSGB.

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

1. While the overall review process is excellent, there is an opportunity to communicate the results of proposal review and the decision-making process more fully with PIs. Specifically, while it was evident that most PMs were reaching out to the PIs of declined proposals with offers to communicate verbally about the results, these efforts were not always documented in the Portfolio Analysis and Management System (PAMS). This made it difficult for the COV to ascertain whether this information was being communicated to PIs. The COV therefore encourages CSGB to discuss what information is appropriate to communicate to PIs about funding recommendations and how those communications should be documented in PAMS. This would serve both as a robust internal documentation assisting the ability of the COV to assess the program, and a standardization of the information communicated with PIs.
2. In discussions with DOE personnel, it was evident that there are multiple pathways that DOE uses to educate potential PIs about BES funding opportunities, mission, and program information. These include, for example, joint webinars with the National Science Foundation and invited talks by PMs at professional meetings. However, the COV felt there may be opportunities to reach a broader audience of researchers. Thus, the COV recommends that CSGB evaluate their strategy for reaching a broad range of potential PIs and educating them about research opportunities in DOE-BES and the unique mission-driven character of BES research. A suggestion that could improve the effectiveness of outreach activities is to advertise informational webinars on the CSGB web-site next to the funding opportunity announcements.
3. In order to maintain a global perspective on new research relevant to their programs and international competitiveness, we encourage continued support of travel for PMs to attend national and international scientific meetings to maintain U.S. and BES prominence in the chemical sciences, geosciences and biosciences.
4. While maintaining the depth of individual programs, it is recommended to continue to develop research across Programs and Division boundaries and/or introduce new capabilities. This could be in the form of thematic PI meetings that cross program boundaries, or formalizing the policy of smaller seed grant opportunities for high-risk, high-reward concepts. Another mechanism could be to expand the Early Career program, and to continue to use it to bring new ideas into the respective programs. The COV recognizes that this may require funding decisions above CSGB's level.

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

1. Given that the COV was conducted for a virtual conference for the first time during this review, the consensus was that this worked, but that in person meetings are preferred because they promote communication and free exchange of ideas. Beyond COV meetings, virtual meetings could be used to augment in-person meetings to preserve travel budgets. This would allow a greater diversity of attendees for PI meetings, e.g., post-doctoral researchers and graduate students.
2. It was evident that there was a heterogeneity in the quality of reviews in some cases. This issue is presumably exacerbated for funding opportunities that were tightly focused on research communities with a small number of qualified personnel in the pool of potential reviewers. The COV thought that CSGB might consider how review quality might be improved in situations where small reviewer pools are expected. These include utilizing a properly curated panel review, or prompting reviewers specifically to delineate strengths and weaknesses in their written reviews.
3. The COV found the supplied materials were extremely useful for evaluating the open solicitation calls for universities, third year renewal of the national laboratory programs and both proposals and pre-proposals for the special funding opportunities (e.g., QIS). However, the initial information supplied for the Early Career Award program was not sufficient for the committee to evaluate the proposal selection process. This was because information about final selections was withheld due to widespread institutional conflicts of interest for the reviewed proposals with COV members. To remedy this, the proposal selection process was reviewed by a subset of the committee members, which presented a tractable number of proposals with institutional conflicts of interest for DOE staff to redact. The requested information was sufficient for the subset of the COV to evaluate the selection process.

## Appendix I: Charge from the Chair of BESAC, Prof. Marc Kastner to the Chair of the COV, Dr. Andrew Stack



December 4, 2019

Dr. Andrew Stack  
Chemical Sciences Division  
Oak Ridge National Laboratory  
One Bethel Valley Road, P.O. Box 2008  
Bldg. 4100, Rm. C346  
Oak Ridge, Tennessee 37831-6110

Dear Dr. Stack:

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 program elements during the fiscal years 2017, 2018, and 2019. The panel may examine any files from this period for both Department of Energy (DOE) laboratory projects and university projects. The Division elements that the COV is being asked to review are:

- (1) Fundamental Interactions
- (2) Chemical Transformations
- (3) Photochemistry and Biochemistry

We will provide background material on these program elements prior to the meeting. The COV is scheduled to take place September 9 – 11, 2020 at the Hilton Washington DC/Rockville Hotel & Executive Meeting Center, Rockville, MD. A presentation to BESAC is requested at its Spring 2021 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.

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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 Runkles, Office of Basic Energy Sciences at 301-903-6529 or by e-mail at [katie.runkles@science.doe.gov](mailto:katie.runkles@science.doe.gov). Teresa Crockett, the BES Program Analyst, will provide logistical support for the COV meeting. She may be contacted by phone at 301-903-5804 or by e-mail at [Teresa.Crockett@science.doe.gov](mailto:Teresa.Crockett@science.doe.gov). For questions related to the Chemical Sciences, Geosciences, and Biosciences Division, please contact the Division Director, Bruce Garrett, at 301-903-8165, or by e-mail at [bruce.garrett@science.doe.gov](mailto:bruce.garrett@science.doe.gov).

Sincerely,



Marc Kastner, Chair  
Basic Energy Sciences Advisory Committee

cc: H. Kung  
B. Garrett  
K. Runkles  
T. Crockett

## Appendix II: COV Members and Contact Information

Last Name	First Name	Institution	Email
Stack	Andrew	ORNL	stackag@ornl.gov
Pyrak-Nolte	Laura	Purdue U	ljpn@physics.purdue.edu
Gaffney	Kelly	SLAC	kgaffney@SLAC.Stanford.EDU
Broderick	Joan	Montana State	jbroderick@montana.edu
McCabe	Bob	NSF	RMCCABE@nsf.gov
Abergel	Rebecca	LBNL	RJAbergel@lbl.gov
Johnson	Paul	LANL	paj@lanl.gov
Soderholm	Lynda	ANL	LS@anl.gov
Walton	Krista	Georgia Tech	krista.walton@chbe.gatech.edu
Gaarde	Mette	LSU	gaarde@phys.lsu.edu
Govind	Niri	PNNL	niri.govind@pnnl.gov
		Washington State	
Clark	Aurora	U	auclark@wsu.edu
Orlando	Thomas	Georgia Tech	thomas.orlando@chemistry.gatech.edu
Mullin	Amy	U Maryland	mullin@umd.edu
Brudvig	Gary	Yale	gary.brudvig@yale.edu
Harwood	Carrie	U Washington	csh5@uw.edu
Gunner	Marilyn	City College U NY	mgunner@ccny.cuny.edu
Beard	Matt	NREL	matt.beard@nrel.gov

### Appendix III: COV Panel Assignments

Last Name	First Name	Institution	Role	Primary Program Focus
Stack	Andrew	Oak Ridge National Lab	Chair	
<i>Panel 1: Fundamental Interactions</i>				
Gaffney	Kelly	SLAC	Panel Chair	
Clark	Aurora	Washington State U	Subject Matter Expert	Computational/Theoretical Chem
Gaarde	Mette	Lousiana State U	Subject Matter Expert	Atomic, Molecular, Optical Science
Govind	Niri	Pacific Northwest Natl Lab	Subject Matter Expert	Condensed Phase/Interfacial Mol Sci
Mullin	Amy	U Maryland	Subject Matter Expert	Gas Phase Chem Phys
Orlando	Thomas	Georgia Tech	Subject Matter Expert	General
<i>Panel 2: Photochemistry and Biochemistry</i>				
Broderick	Joan	Montana State U	Panel Chair	
Beard	Matt	National Renewable Energy Lab	Subject Matter Expert	Solar Photochemistry
Brudvig	Gary	Yale	Subject Matter Expert	General
Gunner	Marilyn	City College U New York	Subject Matter Expert	Photosynthetic Systems
Harwood	Carrie	U Washington	Subject Matter Expert	Physical Biosciences
<i>Panel 3: Chemical Transformations</i>				
Pyrak Nolte	Laura	Purdue U	Panel Chair	
Abergel	Rebecca	Lawrence Berkeley National Lab	Subject Matter Expert	General
Johnson	Paul	Los Alamos National Lab	Subject Matter Expert	Geosciences
McCabe	Bob	National Science Foundation	Subject Matter Expert	Catalysis Science
Soderholm	Lynda	Argonne National Lab	Subject Matter Expert	Heavy Element Chemistry
Walton	Krista	Georgia Tech	Subject Matter Expert	Separation Science

## Appendix IV: COV Agenda

### DRAFT AGENDA Basic Energy Sciences Advisory Committee Committee of Visitors for the Chemical Sciences, Geosciences, and Biosciences Division

**Virtual Meeting  
September 8-11, 2020**

**Zoom sessions will be reserved for 1-5PM on September 8 and 11AM – 4PM other days (all times ET)**

#### Preliminary Activities (Dates TBD)

<b>Time</b>	<b>Activity</b>	<b>Description</b>
Week of Aug 31	Presentation and background material available to COV	Uploaded into PAMS COV module (background information includes BES and CSGB overview, team descriptions, our review processes)
Aug 27, 1:30 – 3:00 PM ET	Zoom training PAMS training	Zoom training by ORISE PAMS training by BES (Jeff)

This draft agenda intends to identify COV activities (reading documentation, deliberating on their findings, writing their reports, and interacting with BES staff). The times are flexible except for presentations the first morning.

#### Tuesday, September 8, 2020

<b>Time</b>	<b>Activity</b>	<b>Description</b>	<b>Participants</b>
12:45 PM	Zoom connections available		All
1:00 PM	Welcome and Charge to the Committee	Presenter: Cynthia Friend (Harvard University) co-Chair of Basic Energy Sciences Advisory Committee	All
1:15 PM	Review presentations/Q&A: <ul style="list-style-type: none"><li>• Basic Energy Sciences welcome/overview</li><li>• CSGB Division overview</li><li>• Proposal Review Process</li></ul>	Presenters: <ul style="list-style-type: none"><li>• Linda Horton, Associate Director, Office of Basic Energy Sciences</li><li>• Bruce Garrett, Division Director, Chemical Sciences, Geosciences, and Biosciences</li><li>• Gail Mclean, Team Lead, Photochemistry and Biochemistry</li></ul>	All
2:15 PM	Instructions and Review of Schedule	Presenter: Andrew Stack(ORNL), COV Chair	All
2:45 PM	Break and move to breakout sessions		
3:00 PM	Panel breakout sessions:	Session begins with a brief overview of the team and its programs by the team	COV, BES, ORISE

	<ul style="list-style-type: none"> <li>• Fundamental Interactions</li> <li>• Photochemistry and Biochemistry</li> <li>• Chemical Transformations</li> </ul>	lead; COV members begin work on reviewing material; BES staff available in the zoom sessions to address questions and provide assistance with PAMS	
4:00 PM	Panel breakout sessions continue	Zoom continues for discussions among COV members; BES staff out of zoom breakout sessions, but available by zoom (holding session), email or phone to address questions	COV, ORISE
4:30 PM	Check-in Meeting between Chair and Panel Leads (panel breakout sessions continue)	Discuss relative progress in panels and observations from discussions and panel check lists/reports; consider any course corrections	COV Chair and Panel Leads; BES leadership if requested
5:00 PM	Adjourn breakout sessions for the day	Zoom ends for the day; panelists can continue to work offline; BES staff available to address questions	

### Wednesday, September 9, 2020

<b>Time</b>	<b>Activity</b>	<b>Description</b>	<b>Participants</b>
11:00 AM	Panels breakout sessions reconvene	COV members continue reading, discussing, and completing panel check lists and panel reports; BES staff available by zoom, email or phone to address questions	COV, ORISE
2:30 PM	Executive Session for all COV – report outs from panels leads on the panel reports	COV discusses output from panels and decides if other work is needed (reading new material, bringing new eyes to old material, ...)	COV, ORISE
3:30 PM	Executive Session for Chair and Panel Leads	Discuss initial panel reports and path forward	COV Chair and co-chairs
3:45 PM	Check-in Meeting with Chair and BES Senior Management	Brief BES Senior Management on progress and have opportunity to ask questions and obtain clarification on any issues	COV Chair, BES leadership
4:00 PM	Adjourn for the day	Zoom ends for the day, panelists can continue to work offline, BES staff available by email or phone	

**Thursday, September 10, 2020**

<b>Time</b>	<b>Activity</b>	<b>Description</b>	<b>Participants</b>
11:00 AM	COV Executive Session	Discuss plan for the day – more time for additional reads to resolve any issues arising from panel reports or move on to finalizing panel reports, summary report and presentation	COV, ORISE
	Panel breakout sessions	Continue reading if needed to finalize/update panel reports; BES staff available by zoom, email or phone to address questions	COV, ORISE
	COV Executive Session	Discuss panel reports, identify key findings and recommendations	COV, ORISE
4:00 PM	Adjourn for day		

**Friday, September 11, 2020**

<b>Time</b>	<b>Activity</b>	<b>Description</b>	<b>Participants</b>
11:00	Writing Session – completion of report		COV, ORISE
TBD	COV Executive Session		COV, ORISE
TBD	Closeout Session with COV and BES	Presentation of key findings and recommendations	COV, BES, ORISE
TBD	Download Clean-up Demo (Apple plus PC)	BES will walk COV members through steps to remove files from personal computers.	COV, BES, ORISE
No later than 4PM	Adjourn		

## **COV Members**

Andrew G. Stack (ORNL)

### Fundamental Interactions

Kelly Gaffney (SLAC), Panel Lead

Mette Gaarde (LSU)

Niri Govind (PNNL)

Aurora Clark (Washington State U)

Thomas Orlando (Georgia Tech)

Amy Mullin (U Maryland)

### Photochemistry and Biochemistry

Joan Broderick (Montana State), Panel Lead

Gary Brudvig (Yale )

Carrie Harwood (U Washington)

Marilyn Gunner (City College U NY)

Matt Beard (NREL)

### Chemical Transformations

Laura Pyrak Nolte (Purdue U), Panel Lead

Bob McCabe (NSF)

Rebecca Abergel (LBNL)

Paul Johnson (LANL)

Lynda Soderholm (ANL)

Krista Walton (Georgia Tech)

## **BES Staff**

Bruce Garrett, Division Director

### Fundamental Interactions

Jeff Krause, Team Lead

Greg Fiechtner

Aaron Holder

Tom Settersten

Wade Sisk

### Photochemistry and Biochemistry

Gail McLean, Team Lead

Chris Fecko

Stephen Herbert

Bob Stack

### Chemical Transformations

Raul Miranda, Team Lead

Chris Bradley

Dan Matuszak

Jim Rustad

Viviane Schwartz

Philip Wilk

## 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?	
Is the research appropriate for the program's 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:	
Pls 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?	
Is the research appropriate for the program's 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:	
Pls national/international leaders in their fields?	

## Appendix VI: COV Report Template and Panel Reports

### 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:

**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 projects and programs.
- (2) Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
  - (a) Breadth and depth of portfolio elements, and
  - (b) 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 contains 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 programs have strong university and laboratory components and, with the exception of CTC, they support both experimental and theoretical/computational work.

Proposals are solicited through the Funding Opportunity Announcement process; program managers do not directly solicit proposals from potential PIs.

The program managers do an excellent job providing substantive and professional reviews. The proposals we looked at were each reviewed by 3-6 reviewers. The vast majority of the reviewers provided substantive assessments of the scientific merit and appropriateness of the proposed approach, relevance to program objectives, experience of the PI, and budget considerations. Program manager assessments clearly focused on the more substantive reviews and clearly considered the merit of reviewer concerns and critiques.

For the open solicitation, the chosen reviewers were appropriate for the projects they were assessing. For responses to targeted funding opportunity announcements, the timeline for the reviews and the extensive conflicts of interest for the many potential reviewers present additional challenges. More specifically, the reviewers do not appear to have the same level of specific technical expertise and knowledge of the BES-CSGB programmatic mission. This influences the reviewers' ability to assess the "Appropriateness of the proposed method or approach" and "Relevance to the Mission of the specific program."

For the majority of proposal reviews, the Procurement Request Package for awards and the Declination Memo for declined proposals provide detailed assessments of the proposals and demonstrate the robustness of the review process. These documents are extremely valuable for the Committee of Visitors process. Additionally, these summaries provide information of significant value to PIs which we assume are shared through informal or other means. These communications to the PIs were not readily accessible to the COV, or do not exist for the Early Career Research Proposals, making the assessment more challenging.

PM transitioning appears to be handled well.

#### **Comments:**

We recommend tracking the demographics of the reviewers, in addition to the demographics of the proposers.

It is critical that the PMs are able to participate in conferences and workshops to remain current on all research related to the programs they support, identify potential new directions, and identify potential reviewers. We strongly encourage the continued support of travel budgets for PMs, and especially the newer PMs as they come up to speed, so that they are better informed about the breadth of the field for their respective programs and the potential for identifying exciting new research directions.

Having an email record that PMs have offered to discuss declinations with PIs would add transparency to the documentation of proposal actions.

In PAMS, the Action History page (under Process) is really helpful to track the timeline of the proposal from submission, review, acceptance/declination. Perhaps links to the Procurement Requests and Declination Memos and other documents can be added here (if possible) to make PAMS navigation easier for future COVs.

#### **Recommendations:**

We recommend a standardization of information included in PAMS regarding the proposal review process and communications with the PI. These would serve as a robust internal record (assisting, for example, the ability of the COV to assess the program).

We strongly encourage the continued support of travel budgets for PMs.

**(b) Monitor active projects and programs. Consider, for example**

- Written progress reports
- PI meetings
- Site visits
- Effective interactions between program managers and PIs

**Findings:**

The Principal Investigators' Meetings Reports provide detailed progress through the PI abstracts for both University and Lab supported PIs. In addition to these Abstracts, University PIs and some of the FOA supported activities also have yearly progress reports. The PI meetings are a valuable means of communication between funded PIs and between the program manager and the PIs. These meetings also are an important mechanism for communicating the evolution of the program mission. The PMs utilize these meetings to communicate and refine the program mission. Separate meetings are run for each of the programs and some PIs whose work cuts across several of the programs are provided the opportunity to alternate between several contractors' meetings or attend more than one a year.

In addition to the PI meetings, it was evident that telephone conversations provide a critical means of interaction between PMs and PIs. This is particularly important for new proposals, where PMs have extended phone conversations with PIs to discuss white papers, as well as funding decisions, both positive and negative. This process has enabled considerable exchange of information. On the other hand, such conversations can be challenged by the human factor in that what is said may not be completely aligned with what is received. With the excellent descriptions of funding decisions already generated by the PMs, we encourage CSGB to evaluate what information from the Procurement Request Packages and the Declination Memos is acceptable to share with the PIs in writing. This is particularly important for proposals that are declined or terminated. For new PI's considering applying to a program, the outreach and engagement activities of the PM's are incredibly important. Reports from site visits are very comprehensive, consistent with the size of the programs, and thorough. When a multi-investigator (>5) on-going project was not continued, detailed, clear, and well-reasoned feedback was provided to the PIs.

Declinations of ECRPs from candidates who are already in a core program are consistently handled.

**Comments:**

We encourage the continuation of annual PI meetings as they are an important venue for interaction, collaboration, and identification of new research directions. We encourage PMs to consider inviting speakers from other programs in BES to stimulate collaboration and potential new directions for programs.

A cohesive and public approach to educate potential PI's about specific programs and opportunities has the potential to keep the programs and PI's current. Webinars, research conferences, and workshops could be used for this purpose. These events could be recorded for

dissemination on the DOE website. While it is evidence that a database of all funded projects exists, it could be more easily located, perhaps by including a link on the CSGB web-site. This would help to educate potential PI's on program scope.

### **Recommendations:**

Develop a plan for reaching a broader range of potential PIs and educating them about research opportunities in DOE-BES.

## **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:**

- Overall quality of the science
- Balance of projects with respect to innovation, risk, and interdisciplinary research
- Evolution of the portfolio with respect to new investigators and new science thrusts
- Relationship of the portfolio to other parts of the Division
- Appropriateness of award scope, size, and duration

### **Findings:**

The program managers are doing an excellent job in actively managing their portfolios. The program managers establish and maintain strong interactions with current and potential PIs through conferences, workshops, PI meetings, phone conversations, proposals, and white papers. This enables them to identify synergies in the expertise of several PIs to develop teams that can pursue science that is impactful and important to the program's mission.

Our findings point to the fact that the PMs are involved in proactive portfolio management with evidence that the PMs know the portfolio well and have a well-articulated vision of the trajectory for the program. We saw evidence that the portfolio management was balanced among innovation and risk and that assessment of renewal awards included an appreciation of long-term program goals. In addition, efforts to maintain and/or improve program vitality and relevance are viewed in a very positive light.

Overall the quality of the science supported by the Fundamental Interactions team is excellent. This conclusion is supported by the program stature documents, the prominence of the publications generated by supported projects, and the highly competitive nature of the proposal award process.

The Early Career Program is essential to increasing the breadth and diversity of the program portfolios and has been successful. It provides a crucial opportunity for program growth and evolution. The focused program calls for small research teams are an effective pathway for increasing the portfolio strength and for introducing new and possibly younger investigators into the program.

The strategic planning within CSGB initiated by Bruce Garrett in 2017 identified five research themes of emphasis within CSGB. These themes are clearly reflected in the program objectives, as well as the areas of research emphasis and de-emphasis. The themes also provide opportunities for synergies between programs. We see value in coordinating the research objectives of the programs within CSGB, between the Divisions in BES, and potentially between Office of Science Programs like ASCR and BER. Two critical needs highlight the importance of identifying and supporting research that crosses program boundaries.

- Many of the most important scientific challenges captured by the BES mission require interdisciplinary and multi-disciplinary approaches.
- Coordinating the activities of the three research divisions within BES (CSGB, MSE, and Facilities) with the infrastructure investments primarily in the Facilities Division (Nano-Centers, x-ray light sources, and neutron facilities) will be increasingly important as international research competition continues to increase.

### **Comments:**

The success and vitality of the programs depend on the commitment, expertise, and enthusiasm of the PMs. Career development, such as cross-training between programs and teams, could assist the identification of new research directions that naturally leverage the strengths of the existing programs.

Consider expansion of the Early Career program in terms of number of awards at both the laboratories and universities. The panel realizes this is a decision made above CSGB within DOE.

Continue to support small research teams to pursue new directions and introduce new collaborations within and across Programs and Divisions. This could be in the form of smaller seed grant opportunities for high-risk high-reward concepts.

### **Recommendations:**

Continue to create incentives for identifying and supporting (1) research collaboration across Program and Division boundaries and (2) new and early career PIs that will enhance the vitality of the programs.

### **(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 programs have internationally-recognized impact in their areas of emphasis. The mission focus of the programs ensures the distinctive character of the Fundamental Interactions Team

programs.

The programs support a very strong group of PIs at various career stages. There is an impressive group of younger researchers, with several of the younger faculty receiving Sloan and other early career awards. Mid-career and senior researchers and faculty have received a variety of prestigious awards and recognition, including election to the NAS and ACS national awards.

The PIs are also active in the community as editors of the top journals in chemical physics, physical chemistry and AMO physics. They are also actively engaged in conference and workshop organization.

All programs described high-impact outcomes of funded work.

**Comments:**

The research landscape continues to evolve rapidly with competition and collaboration crossing national boundaries. It is essential for BES CSGB, and the PIs whose research is supported, to be fully cognizant of research progress in Europe and Asia. Inviting leading researchers from outside the programs and the US to speak at PI Meetings could provide valuable feedback on the program and PI standing internationally. Small funding opportunities to support conferences in the US with broad constituencies should continue to be supported.

**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 section of CSGB integrates research projects that span Biology, Chemistry, and Physics, and is organized into three programs: Solar Photochemistry, Photosynthetic Systems, and Physical Biosciences. All three programs fund research at both universities and national laboratories. The three programs have strong synergy directed towards the goal of understanding the fundamental mechanisms of solar energy capture, conversion, and storage through biological and chemical pathways. This goal is critical to the DOE mission. The presence of these programs within CSGB serves to provide insight to the more physical science-oriented divisions as to how biology carries out certain difficult chemical processes – for example light-energy capture and nitrogen fixation – relevant to energy capture, conversion, and storage. These mechanisms may provide a blueprint for how to accomplish these processes in artificial systems.

Overall, the COV finds the proposal solicitation and review process to be excellent. Three or more reviewers with appropriate expertise provided reviews for each proposal, and in most cases

the reviews were substantive. The funding recommendations made by the Program Managers were generally well-supported by the reviews, consistent with the program mission, and were often documented in PAMS with detailed selection statements. It was clear to the COV that great care is taken in the review process by the Program Managers. In some cases, strategic decisions were made without strongly supportive reviews in order to facilitate the development of new methods or systems with potential for transformative results. The deep engagement of the Program Managers, their knowledge of the field, and the flexibility they have to shape their respective programs in a way that strikes a balance between mission focus, development of a diverse group of PIs, and establishment of a community of PIs with common goals in pursuing fundamental research is the foundation of their successful, forward-looking, and far-reaching programs.

Proposal review panels are used by Photosynthetic Systems and Physical Biosciences, and were viewed favorably by the COV. The panel discussion can improve the quality and scope of the review process, though their purpose is not to reach a consensus. They provide input to both the PI and the PM, and the additional information that emerges from the interaction between the reviewers during the panel can be particularly valuable.

In reviewing the pre-proposal process via documentation provided in PAMS and through discussions with Program Managers, the COV finds the process to be effective. The flexibility of this process, and the ability of potential PIs to discuss their research ideas with Program Managers to determine whether they fit in the program, is good for the program and for PIs. Although this process works for PIs with experience with BES, it may miss potential PIs who are not as familiar with the DOE and its programs.

The COV noted that the mix of funded PIs at different states of their career is a strength, and the Early Career program plays an important role in this. Although only limited information was available regarding the Early Career selection process, it seems to be working well. The down-select process for pre-proposals involving all three PMs strikes a good balance between fairness and making the process manageable. It would be helpful to provide a better “paper trail” in PAMS on the review process. Although feedback is often appropriately provided during phone calls, the information in PAMS often did not provide a clear picture of what was done and when. Part of the problem is that PAMS is not very user friendly, and this could be improved.

The COV views the use of terminal awards as a strength of the program that should be continued. It allows PIs to complete and publish their findings, and allows project personnel to move on in an orderly fashion. Terminal awards also allow the PM to have the flexibility to shape their program.

### **Comments:**

The COV would like to see PAMS continue to evolve to become more user-friendly, so that it is less cumbersome for Program Managers to document communications with potential PIs in the pre-proposal phase of discussion about possible grant proposals. At the same time the COV does not want to hinder the flexibility of Program Managers or to make this an onerous task. Overall,

it is important to balance the need to retain a record with allowing the program managers to have a free exchange of ideas with the scientist who is trying to obtain funding.

### **Recommendations:**

The COV recommends that panel review of proposals be supported as much as possible, in order to maintain the high quality of the review process and the feedback provided to PIs. The make-up and function of review panels can be tailored to meet the PM's goals and needs.

The COV recommends that reviewers be specifically prompted to delineate strengths and weaknesses in their written reviews of proposals, in order to provide more uniform, substantive and clear reviews for PIs and PMs. This could be done by having "strengths" and "weaknesses" subheadings in the sections of the review form, for example. Alternatively, each reviewer could be asked to write a summary statement that clearly describes strengths and weaknesses. In the absence of a written summary statement of the review from the PM for the PI, it becomes more important for clear summary statements from each reviewer. This is particularly important information for PIs whose proposals are declined.

The COV recommends greater exposure of outreach activities to potential PIs, for example via webinars, to provide more insight into DOE programs, funding opportunities, and the process of proposal submission and review.

### **(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 written progress reports are a useful tool for Program Managers to monitor PI progress.

The COV views PI meetings as highly valuable, both for the ability of PIs to talk directly to Program Managers, and for PIs to interact with others in the program. The program benefits from the collective breadth of the PIs, and the meeting helps to seed new collaborations. An exceptional strength of this program is that it brings together PIs with expertise in biological and physical sciences. This can lead to collaborations within the program, thus generating novel interdisciplinary research directions. The PI meetings help to build a sense of scientific community in the program. They are a feature that make DOE funding unique and uniquely valuable.

The multifaceted interactions between Program Managers and PIs are highly effective and important for the programs. Through PI meetings, phone calls, and interactions at scientific conferences, the Program Managers provide critical and regular feedback to PIs on the mission-

driven relevance of their research, and in turn are open to input from their PIs to shape their programs.

### **Comments:**

The COV notes that the Program Managers are active and very effective at determining when projects are unproductive or drifting outside of the program mission. Program Managers take great care to clearly communicate their concerns and expectations to the PIs, especially in advance of project renewal proposals. The one year of funding provided to terminated projects was viewed favorably by the COV.

The current three Program Managers work very well together with Dr. McLean anchoring an excellent team. The interactions amongst the PMs leads to a flexible and open approach to funding with proposals moving between programs and PIs being comfortable to approach different Program Managers for advice.

### **Recommendations:**

The COV recommends that Program Managers continue to be supported to attend key scientific conferences, whether in-person or virtual. These conferences provide an important opportunity for PM – PI interactions, and also allow the Program Managers to evaluate the greater breadth of related scientific disciplines as they guide their programs towards the greatest mission-relevant impact. In addition, as the programs are portfolio-driven with different areas losing or gaining importance, the informal talks with Program Managers at conferences help to disseminate these shifts to the community.

With regard to program meetings, cross program participation could be increased by inviting PIs from other programs to attend program meetings where overlap exists, for example Photosynthetic Systems and Solar Photochemistry. Allowing some participation from promising postdocs and graduate students could be also be beneficial.

## **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 COV found the quality of the research to be exceptional across all three programs. The portfolios are well-balanced with respect to research area, innovation, and risk. The program managers clearly have the ability to fund high risk/high reward proposals and to take the time to see how they progress. The programs are clearly differentiated and have good synergy. The Program Managers work effectively to continually evaluate the focus of their own programs to encompass the most exciting and mission-relevant science. As the Program Managers reshape the research priorities and directions of their programs, it is important to ensure that subtle changes in mission are clearly communicated to the PI community and beyond. The PMs accomplish this through carefully crafted mission statements, one-on-one discussions, portfolio presentations at PI meetings, and informational sessions at other scientific meetings. The PMs work well together and there is also evidence of good collaboration with other parts of the Division.

Another beneficial element is the balance of new and established investigators. The addition of new investigators adds new research areas into the programs. At the same time, the practice of continuously funding established and productive investigators provides a mechanism to allow fields supported by the DOE to develop. The choices of the program managers to fund some exploratory research also invigorates the program.

Early Career awards provide an additional funding mechanism to bring exciting new investigators into the program. This program also provides a pipeline to identify promising PIs to add to the core program.

The COV agreed that the Program Managers are doing an excellent job of maintaining vibrant programs within the limitations associated with their budgets. Given the budgetary constraints, the awards are appropriate in size, scope, and duration.

The use of strategic planning, BRNs, and other community outreach in order to help shape and define core programs is very useful and appears to be of great help to the PMs, PIs, and prospective PIs.

**Comments:**

The COV appreciates the Program Managers' efforts to find other funding mechanisms for promising new grants that don't fully satisfy the Early Career program.

**Recommendations:**

Continued ability of PMs to attend a range of scientific conferences relevant to their program, whether in-person or virtual, is essential to the vitality and continued success of the programs. The COV recommends that these activities continue to be supported for the PMs.

**(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 research in the three programs in Photochemistry and Biochemistry fills an important niche relevant to the DOE mission and is distinct from research programs funded by other agencies. The integration of questions and methodology from Biology, Chemistry, and Physics to understand the fundamental basis of solar energy capture, conversion, and storage in photosynthetic systems provides for highly novel and synergistic science that supports the overall DOE mission. The COV finds that there is an appropriate balance of proposals to develop new tools with those focused on hypothesis-driven research. This is a welcome element of the portfolio.

The program PIs are high-profile, respected scientists both nationally and internationally. They include members of the National Academy of Sciences and National Academy of Engineering, distinguished fellows of scientific societies, and winners of the top prizes in science, including a Nobel Prize winner. They hold key leadership positions as editors of top journals and organizers of the most important national and international conferences in the field. The gender balance has improved in the group of PIs.

**Comments:**

None

**Recommendations:**

The impact of programs in CSGB could be more broadly appreciated with promotion of the scientific output of the programs both to the scientific community and also to the greater society. BES Highlights are a fantastic avenue but are not as well known to those outside of DOE. In addition, the recent report on how BES science has impacted society is great and could be promoted and perhaps expanded in future installments.

**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:**

Recent strategic planning efforts have resulted in a clear description of the general research priorities within this program, which are well documented and available through a variety of avenues, including the BES reports, BRNs, and individual program webpages.

The portfolios contain top-notch researchers who conduct cutting-edge research that falls within the Office of Science CSGB mission. The solicitation of relevant proposals for the Chemical Transformations team is very strong for the open solicitations but a number of non-relevant pre-proposals are submitted to the Early Career program.

The review and recommendation process is rigorous and impressive in most cases. The PMs work diligently to find qualified and mostly constructive reviewers, and put tremendous effort into the synthesis of multiple reviews into impressive funding recommendation statements. In many cases, a PM was found to have conducted additional reading on a topic that enters into the decision.

The documentation procedure for decisions was found to be very strong in most cases. However, a lack of uniformity in the types of information funding decisions the COV found on PAMS was sometimes observed. Whether this is due to different types of information included in PAMS (or perhaps stored in different locations), or variation due to the nature of the solicitation or difficulty of the award or declination was not clear.

The Chemical Transformation team evolved their topical areas through strategic planning that has led to de-emphasis of certain topics and emphasis of support on new and emerging topic areas. For instance, CSGB efforts to incorporate data science into the program's portfolio over the last two years will have long term benefits to the scientific community and are a model for other agencies.

For some declined proposals, the scientific reviews often provided an array of positive and negative comments, but how these comments were weighted is not communicated to PIs. However, the weighting is extremely clear from a PM's internal declination letter. While it is clear that DOE refrains from commenting on the rationale for a funding recommendation in documents provided to PIs, it is not always documented that the PMs communicated a willingness to discuss the results by phone.

The Early Career pre-proposals are screened for alignment with program thrusts and technical merit by panels of 3 program managers. This involves a significant commitment of program manager time, but also places an intellectual burden on the program managers to bring a deep level of technical expertise to each pre-proposal. The breadth of some programs is such that a PM panel may not immediately have the technical expertise to judge the merit of the pre-proposal, especially given the restricted "space" allotted the investigator to fully explain and support the proposed concepts. The result may be an undue intellectual burden on the PM panels, but whether the practice results in a net reduction in effort is unclear since this also reduces the workload during proposal review.

### **Comments:**

CSGB is doing an excellent job in soliciting proposals from new and current researchers, has an excellent review and recommendation process because of the high quality of the PMs, and has good documentation of the review process/actions.

### **Recommendations:**

Evaluate mechanisms to inform potential Early Career proposal writers about the mission of CSGB, the topical areas (focus, emphasized versus de-emphasized areas), and other information that will aid the solicitation of relevant research topics that lead to quality proposal submissions. The mechanism should provide a method for potential applicants to ask clarifying questions. (For instance, such a mechanism could be an online town-hall style presentation.)

For declinations, the post review communications should make clear to a PI that they are encouraged to discuss the decision with the PM if the scientific reviews do not provide sufficient

insight into the decision.

The COV recommends that CSGB look for an additional approach to supplement the pre-proposal panel review when needed with a subject matter expert directly related to the pre-proposal.

It was evident CSGB experts carefully considers multiple factors during proposal review while making funding recommendations, it was thought that CSGB should consider ways to communicate that effort to PIs. Examples might include creating a guidance letter for university projects, ensuring funding recommendations communicated to PIs include offers to discuss results (and is documented in PAMS), or review the factors that inform funding recommendation decisions.

**(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 PMs do an excellent job in monitoring active programs through fabulous PI meetings that also offer a great venue for peer-to-peer interaction and evaluation.

University renewal grant folders contain yearly progress reports and a progress section within the proposal. Most reports are concise but thorough and appear to be useful in the assessment of progress during grant period. It appears that laboratory programs do not have a requirement for regular progress reports, but renewal proposals include sections on past performance within the proposals. For renewal and lab proposals, reviewers and program managers often refer to progress made in previous grant periods in their evaluations.

PI meetings occur at different frequencies depending on the size of the program. They appear to be one of the main, if not only, in person communication channel among PIs from the same program and between the PM and PIs.

PM travel to scientific conferences has increased since the last COV and provides more opportunities for in person discussions with PIs and helps to keep the PMs abreast of the current trends.

PI meetings and PM travel are two extremely important mechanisms to build scientific communities within each program, foster collaborations, and increase creativity and productivity.

Site visits occur during Laboratory program reviews that are comprehensive, include carefully selected panels of reviewers, and are well reported on (mostly under the form of slide decks).

Most interactions between PIs and PMs seem to occur by email or phone, in addition to PI meetings and occasional scientific conferences. For both university and laboratory PIs, this seems to make for efficient and communication with their respective PM.

### **Comments:**

The panel found that the increase in the travel budget had a positive impact on the program and enabled the PMs to interact more often and in person with their program's PIs and with other non-DOE funded researchers, and to provide opportunities to place their programs in context of the broader scientific community. The PI meetings are sufficiently valuable in the formation of scientific communities around each program that the panel expressed some concerns about developing similarly efficient virtual meetings during the COVID-19 pandemic and rapidly returning to in-person meetings once feasible.

### **Recommendations:**

Hold PI meetings with some concurrent sessions for programs with related topics (for example heavy element chemistry and separations, or a cross-program machine learning meeting, and relevant EFRC & HUB presentations.)

Ensure PMs can attend as many virtual conferences as reasonable during the COVID-19 pandemic.

PMs should have the opportunity to attend international conferences or be encouraged to have international speakers at PI meetings to broaden the global perspective of their programs.

Explore new tools to possibly leverage virtual PI meetings during the COVID-19 pandemic to start to include graduate students and postdocs that may not be able to travel to in-person PI meetings in normal times.

Sustain the travel budget and prepare for a rapid and efficient return to in-person meetings when feasible for the PI meeting and for the PMs to attend.

## **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:**

CSGB continues to maintain portfolio elements with excellent breadth and depth. The overall quality of the science and the principal investigators is very high.

PMs have successfully balanced the mission-oriented nature of DOE with the flexibility required to pursue transformative fundamental science, which is a world-class hallmark of DOE-funded research.

PMs have successfully balanced the evolution of their portfolios with respect to new PIs and new science thrusts, while phasing out older (but very successful) topic areas that are no longer aligned with the mission of their portfolios.

PMs do an excellent job in tapering off funding for projects that have been terminated, where there is a need to fund post-docs and students.

CSGB is actively promoting new and emerging areas to expand its breadth while maintaining its depth. CSGB does an excellent job of maintaining depth through long term funding of PIs. CSGB is increasing its breadth through the aggressive approach taken on strategic planning and cross program-cutting themes. For example, CSGB's incorporation of data science into the program is impressive and has led to significant scientific impact well beyond the CSGB program.

CSGB co-sponsored international meetings (e.g. Machine Learning in the Geosciences, 2018 & 2019) maintain the depth and increase the breadth of the program, while increasing CSGB's presence on the international stage and stature.

### **Comments:**

Changing the portfolio complexion requires a delicate balance between judging long-term PI productivity vs. mission drift, and the PMs are commended for proactively growing their programs in exciting directions that naturally encourage the interest of new investigators.

### **Recommendations:**

PMs are encouraged to seek out new ways to maintain PI diversity within their programs by increasing the number of people exposed to CSGB research and programs. This might include leveraging PI meetings, creating new virtual meetings for program introductions, and attendance of PMs at national/international conferences of relevance to their areas.

All CSGB PMs could hold a joint virtual meeting (e.g. town hall style) that is broadly advertised through their respective communities to promote the breadth and depth of their programs, and

may also include select PIs to present substantive short presentations of CSGB-funded work. While subsequent conversations with DOE BES staff showed that CSGB does indeed hold webinars joint with the National Science Foundation, they rely on NSF for advertising and it may be more effective to simply have CSGB display these activities prominently on their own website.

**(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 general, PIs supported by the Chemical Transformations programs represent the best that U.S. universities and national laboratories have to offer. The PIs recognize emerging trends in their fields (not just in the U.S. but globally). The CSGB research portfolio is competitive with other U.S. agencies, and clearly leads in some areas related specifically to energy (e.g., heavy element research, solar energy and geomechanics).

CSGB's aggressive incorporation of Data Science in the program has poised them as the lead agency for machine learning in the geosciences, separation and catalysis fields. The chemical transformation team's foresight on Data Science has positioned them to be the leader in machine learning CSGB topical areas. The Data Science portfolio PIs lead the US and world in proposals of data science to geosciences and chemical sciences problems. The funded geosciences PIs are highly competitive in the US and in many case are leaders in their respective fields worldwide.

**Comments:**

The CSGB is doing a very good job in funding cutting-edge research and individuals with stature at the national and international level.

**Recommendations:**

A mechanism to ensure the maintenance of the CSGB stature is to expand the Early Career program, and to continue to use it to bring new ideas into the respective domains. This may require funding decisions above CSGB's level.