



U.S. DEPARTMENT OF
ENERGY

Office of
Science

**FY 2020 Report of the Committee of Visitors
BES Division of Chemical Sciences, Geosciences,
and Biosciences (CSGB)**

FY 2017, 2018, 2019

September 8-11, 2020

Conducted over Video Conference

Presented to the Basic Energy Sciences Advisory Committee

Andrew G. Stack, COV Chair

December 9th, 2020

Committee of Visitor Charge (Standard)

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.

Solicitations Covered

- FY 2017-2019 Continuation of Solicitation for The Office of Science Financial Assistance Program
- New/Renewal proposals from National Laboratories
- FY 2017-2019 Early Career Research Program
- FY 2017, 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
- FY 2018, 2019 Materials and Chemical Sciences Research For Quantum Information Science
- FY 2019 Data Science for Discovery in Chemical and Materials Sciences
- **Not considered:** the Energy Frontier Research Centers (EFRCs); Fuels from Sunlight Energy Innovation Hub

FY 2020 CSGB Committee of Visitors Composition

- COV membership was selected by the COV chair, Dr. Andrew Stack, in consultation with BES staff and panel leads
- Represents a cross-section of experts in scientific fields relevant to the activities supported by the CSGB Division
- COV Demographics
 - 18 COV panelists organized into 3 panels
 - 10 from academia, 7 from DOE labs, 1 from other Federal Agency (NSF)
 - 9 female, 9 male
 - 12 funded by CSGB
 - 4 served on prior COVs
 - 2 BESAC members (Stack, Broderick)

Three Panels

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

Separation Science

Heavy Element Chemistry

Geosciences



Panel Structure and Membership

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	Louisiana 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

COV Materials

COV members had access to a selection of proposals that had actions (awarded, declined, or withdrawn) in fiscal years 2017, 2018, 2019

Material provided:

- Reference Materials
 - List of total actions: awarded, declined, and withdrawn proposals
 - Program stature documents
- Solicitation Folders
 - Pre-proposal review (for ECRP, QIS, Data Science)
- Proposal Folders
 - Proposals
 - Reviews
 - Declination memos
- Award Folders
 - Budgets
 - Selection statements

COV Agenda

Day 1

- Welcome and charge to COV by BESAC, BES and CSGB overviews
- Panel breakout sessions: brief portfolios overviews from CSGB team leads; first read of selected packages by COV; Program Managers on call
- Check-in meeting between Chair and Panel Leads

Day 2

- Panel break out sessions reconvene
- COV Executive session: Report out by Panel Leads on Preliminary Findings
- Check-in meeting between Chair and Panel Leads

Day 3

- Executive session: Plan for the day
- Panel breakout sessions: Consider pre-proposal review, ECRP proposals

Day 4

- Executive session: finalize draft panel reports
- Closeout session between COV and BES: presentation of major findings and recommendations

2020 CSGB COV Summary

- Five Major Findings
- Four Major Recommendations
- Three Other Comments and Suggestions



Major Finding 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.**

Major Finding 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 research program proposals** 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.

Major Finding 3

- **CSGB utilizes a diversity of methods** for review 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.
 - E.g., a three-program manager down-select was used in FY19 for 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.
- Overall, the **COV encourages the continued use of a diversity of different methods** for pre-proposal and proposal review where appropriate.

Major Finding 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.
- They are a feature that make **DOE funding unique and uniquely valuable**.

Major Finding 5

- 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.
- 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 themes.

Major Recommendation 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).
- 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.



Major Recommendation 2

- 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.**
- 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 website next to the funding opportunity announcements.

Major Recommendation 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.

Major Recommendation 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.

Other Comments and Suggestions 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.

Other Comments and Suggestions 2

- It was evident that there was a **heterogeneity in the quality of reviews** in some cases (e.g., subject matter experts vs. familiarity with BES priorities).
 - 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 included utilizing a properly curated panel review, or prompting reviewers specifically to delineate strengths and weaknesses in their written reviews.

Other Comments and Suggestions 3

- The supplied materials were extremely useful for evaluating the open solicitation calls for universities, renewal of the national laboratory programs and both proposals and pre-proposals for the special funding opportunities (e.g., QIS).
- Initial information supplied for the Early Career Research Program was not sufficient for the committee to evaluate the proposal selection process. Information about final selections was withheld due to widespread institutional conflicts of interest for the reviewed proposals with COV members.
- To remedy this, **the final ECRP proposal selection process was reviewed by a subset of the committee members**, that presented a tractable number of proposals for DOE staff to redact.
- The requested information was sufficient for the subset of the COV to evaluate the selection process.

Special Thanks

- Bruce Garrett, Director of CSGB
- Raul Miranda, Gail Mclean, Jeffrey Krause, CSGB Team Leads
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- DOE & ORISE Staff (Theresa Crockett, Linda Severs)
- COV Members