## Report of the 2020 Committee of Visitors Division of Chemistry National Science Foundation

Meeting Dates June 1-3, 2020

# Submitted on behalf of the Committee by Peter K. Dorhout, Chair

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### I. Executive Summary

**Recommendation 1: The Division of Chemistry Budget needs to be increased significantly to meet the needs of the community and the nation.** The Committee of Visitors (COV) believes that the Division (CHE) is an excellent steward of the funds it receives. The Division is also active in, and successful at, securing co-funding to increase its ability to support transformative science. However, the combination of flat overall budgets, participation in Foundation-wide initiatives, and increasing costs to PI is leading to a tipping point for chemistry funding for the Division. Excellent science goes unfunded each year. An NSF award "buys" fewer person hours, trains fewer people, and limits the number and impact of critical new findings. Support of the core chemistry research that is the heart of CHE is at risk of being contorted as the community attempts to fit into top-down initiatives. Finally, creative risk-taking science is hampered by short award durations. The Division can advocate for resources on behalf of the chemistry community, but this recommendation is aimed squarely at the Foundation and its ability to expand its overall funding.

**Recommendation 2: Further the impressive moves towards transparency in the review process.** The 2016 COV recommended that the Division work to enhance the transparency of the review process. The current COV finds that considerable progress has been made. Panel reviews and summaries are substantive and communicate reviewer and panel rationales. The Program Officer (PO) Review Analyses (RA) are clear, detailed, and persuasive. The COV found somewhat greater variability in the quality of ad hoc reviews, but they do not comprise the majority of the review portfolio and did not generate deep concern. The thrust of this recommendation is that the COV would like to see PO comments and feedback to PIs expand to include more of the constructive information contained in the RAs. The COV believes PIs would benefit from the PO comments that provided the sort of detailed and reasoned discussions contained in the RAs, because this would not only enhance transparency, but also provide PIs with greater guidance for future submissions.

**Recommendation 3: Employ panels in the review process when possible.** The COV finds that the panel process provides excellent feedback to PIs. The Division currently does the bulk of its reviewing by panel, and the COV urges that panels continue to be central to the efforts of CHE. In addition to the benefits to PIs, panels also serve to acculturate new PIs and provide important networking opportunities. Some concerns were raised about the time commitments required of in-person panels on faculty, but other COV members felt that PIs could decide for themselves, and that in-person panels should remain the norm. The COV also urged the Division to seek broader participation from the community in the review process especially noting a desire to enhance the diversity of its reviewers across the many dimensions of diversity. The COV asks that the Division find ways to engage the community in a discussion of panels and the challenges and opportunities they present.

**Recommendation 4: Seek greater community clarity with respect to Broader Impacts.** The COV believes that Broader Impacts are a critical part of the assessment of proposals to the NSF. However, the COV found that the attention paid to Broader Impacts by reviewers and panels varied considerably across the proposals we examined. Further, it was sometimes unclear how the assessment of Broader Impacts factored into the funding decision. The community as a

whole has widely varying perceptions of what Broader Impacts are, and how to fulfill them. Finally, the COV believes that the ability to assess Broader Impacts lags the ability to assess Intellectual Merit. The chemistry community seeks guidance and education on this issue, since it is clear that confusion persists among proposal writers and reviewers. The COV suggests that the Division find ways to engage the community in discussions about the Broader Impacts and perhaps use these conversations to further educate the community and generate clarity around what they mean to everyone. For example, a series of workshops should be held, out of which community consensus might emerge. Community norming of this type would be of immense benefit to young PIs and also be helpful to reviewers and POs who are asking those reviewers to assess proposals.

**Recommendation 5: Continue efforts to promote inclusion for the scientific enterprise.** The 2020 COV echoes the 2016 COV with this recommendation. The Division should continue outreach to institutions that educate historically underserved populations and primarily undergraduate institutions. The COV recognizes that there may be ways for the Division to promote cross-institution mentoring for PIs at small institutions, where their expertise is singular. The COV recommends that the Division encourage and facilitate a new generation of organizations that promote inclusion at the faculty level. As an example, the Division could promote a database of all new hires in chemistry-related departments across from across the country so as to develop formal and informal networks that continue to support and mentor women and PIs from under-represented backgrounds beyond the impressive CAREER workshop the Division holds. The COV recognizes that many of the most creative ideas have come from the community, which is an essential partner with CHE in order to improve access and inclusion, and it would welcome opportunities to be active participants to support these efforts.

### II. Background

The Committee of Visitors (COV) for the Division of Chemistry (CHE) met virtually for three days (June 1-3, 2020) to review the activities of the Division for the four-year period 2016-2019. Appendix A lists the members of the COV. The forty-four members include the Chair, Peter Dorhout, the co-chairs, Malika Jeffries-EL and Robert Cave, a liaison representing the Directorate of Mathematical and Physical Sciences (MPS) Advisory Committee, William Tolman, and prominent scientists from academia, industry, government laboratories, and other federal agencies (see Appendix A.)

The FY 2020 Division of Chemistry (CHE) COV was charged to address and prepare a report on:

- The Division's response to the prior COV report of 2016;
- The integrity and efficacy of procedures implemented to solicit and review proposals, and processes used to recommend and document proposal actions;
- The quality and significance of the results of the Division's programmatic investments;
- The relationship between the portfolio and the Missions of the Division, the Directorate, and the Foundation; and
- The Division's engagement in, and prioritization of, research initiatives.

In May 2020, prior to the meeting of the COV, several video teleconferences were conducted to prepare the COV members for the review process. These teleconferences were conducted by the CHE Acting Division Director, Dr. Carol Bessel, Dr. Anne-Marie Schmoltner, Acting Deputy Division Director, and other members of the CHE staff. The presentations included a discussion of conflicts of interest and confidentiality, a tutorial on how to access proposals that were awarded and declined in the NSF eJacket System, and Divisional data, including the number of proposals received, reviews requested and received, and funding rates among several demographic categories. The COV members were also provided with the 2016 COV report and the CHE responses to it over a four-year period. After the introductory teleconferences, the COV members were given two additional briefings on data for two different programs, according to the assignments for each member, by the CHE program leads.

The COV meeting began on June 1, 2020 with a welcome by Acting Assistant Division Director for MPS, Dr. Sean Jones, who also presented the charge to the COV. Chemistry Division Director David Berkowitz, and COV Chair Dr. Peter Dorhout welcomed the members and these remarks were followed by a short briefing on conflicts of interest (COIs) by Dr. Kathy McCloud.

The thirteen programs or initiatives that were reviewed include:

- Chemical Catalysis (CAT)
- Chemistry of Life Processes (CLP)
- Chemical Measurement and Imaging (CMI)
- Chemical Structure, Dynamics, and Mechanisms- A and B (CSDM- A and B)
- Chemical Theory, Models and Computational Methods (CTMC)
- Environmental Chemical Sciences (ECS)
- Macromolecular, Supramolecular and Nanochemistry (MSN)

- Chemical Synthesis (SYN)
- Centers for Chemical Innovation (CCI)
- Research Instrumentation Program and Facilities (MRI and facilities)
- Research Experiences for Undergraduates Sites (REU)
- Special Projects and Initiative Investments (combined with REU for the COV)

Each of the co-Chairs of the COV had conflicts with one or more of the 13 programs, and those were managed through the NSF COI management process by limiting access to program eJackets and limiting participation in specific discussion groups. All three co-Chairs of the COV had a conflict with the MRI and facilities program. In order to manage the discussions and prepare a report, one member of the COV, George Schatz, was assigned to provide guidance to the MRI COV discussion section and the compilation of that section of the report.

On the first two days of the COV, each group or subpanel was provided with access to a selected number of proposals (jackets). The jackets were selected to represent a number of clearly fundable cases, clear declinations, and a set of borderline award and declination cases. If subpanels requested additional jackets for review, these were promptly provided following a review for conflicts of interest. Each COV member was assigned to a subpanel according to their primary sub-discipline of chemistry. Each member was also assigned a second subpanel performing a "cross-read" review. During both sessions, the Program Officers (POs) were accessible to COV members. In addition to the individual subpanel meetings, the entire COV met in several sessions to discuss preliminary findings, explore issues and propose recommendations. During this time, the CHE Division Director, Deputy Division Director and Program Directors were available to answer questions from the committee.

On the afternoon of the second day of the COV the members were placed in discussion groups to consider the three "Portfolio Questions" (see Appendix F.) The Chair and co-chairs of the COV facilitated these discussions with the assistance of scribes. Two sessions were conducted, and COV members were asked to select the two questions of greatest interest to them. All those who responded were placed in their first and second choice groups. Other members were assigned to groups randomly. (See Appendix G for a list of the participants in the Portfolio Questions panels.) A summary of these discussions, including dominant themes, was prepared the following day (Appendix H.)

On the third day, the COV discussed the major findings of their work and the Chairs finalized the Report and a presentation on the COV's findings. The Chair presented the results to Dr. Sean Jones and the Division of Chemistry. Following the presentation and ensuing discussion, the COV was adjourned with thanks.

### III. Specific Results of the Review

### A. Integrity and Efficacy of Processes

**1. Review Process** 

The COV believes that appropriate review processes are used to guide funding decisions. The COV viewed panels as a particularly important and valuable part of the review process. The emphasis on panel reviews from during 2016-2019 appears to be a positive response to comments made about the review process by the 2016 COV. The vast majority of comments show that the 2020 COV is supportive and appreciative of how each program is managed; panel reviews and summaries are substantive and communicate reviewer and panel rationales. The Program Officer (PO) Review Analyses (RA) are clear, detailed, and persuasive. The COV found somewhat greater variability in the quality of ad hoc reviews, but these do not form the bulk of the review portfolio and did not generate deep concern. The COV believes that, while PO comments to the PI are generally substantive, they would like to see more of the RA's content shared with the PI.

The COV believes that Broader Impacts are a critical part of the assessment of proposals to the NSF. However, the COV found that the attention paid to Broader Impacts by reviewers and panels varied across the proposals and programs that were examined. Further, it was sometimes unclear how the assessment of Broader Impacts factored into the funding decision. The community as a whole has widely varying perceptions of what Broader Impacts are, and how to fulfill them. Finally, the COV believes that the ability to assess Broader Impacts lags the ability to assess Intellectual Merit. The chemistry community needs education on this issue, since it is clear that clarity has not yet been achieved.

### 2. Selection of Reviewers

The COV believes the programs use reviewers who have the expertise to evaluate the proposals they receive. The 2016 COV recommended that PIs establish databases of reviewers so that reviewer expertise and proposal topic can be mapped properly. Several programs have such databases and the COV believes they should continue to be maintained.

Reviewer diversity continues to be a challenge for the Division, but not for lack of trying. The COV believes the community needs to support the Division in its efforts at Inclusion and would welcome initiatives to partner with CHE.

### 3. Program Management

Consistent with comments made above concerning the review process, the COV believes the programs are well-managed. The POs choose quality reviewers, the panels are encouraged to give excellent feedback, and the PO comments have progressed so that they help PIs understand the rationale for decisions.

The COV believes the programs maintain a good balance among sub-disciplines in their field and that panels are able to assess proposals effectively that span these sub-disciplines. We also believe that the programs are responsive to emerging trends in the field and often fund transformative science. In considering program management the COV's comments are, overall, positive, complementary, and encouraging.

# **B.** The CHE Portfolio and Performance in Contributing to the Strategic Goals of the Division and Foundation

The COV was asked to consider three "Portfolio Questions" related to the Division's stewardship of resources, partnership with the Directorate and Foundation, and interactions with the community as the Division develops new initiatives. These discussions occurred at the end of the COV session on its second day, Tuesday, June 2. Each COV member was assigned to two of the three questions based on selected preferences. One of the Chairs of the COV facilitated the discussion of each of the questions, and a COV member was chosen to scribe the session. The scribes and other discussion participants for the given question then met on the morning of the third day of the COV, Wednesday, June, 3, to merge the responses and capture the groups' recommendations. The full text of the prompts for these discussions is given in Appendix F, and the complete responses from the groups considering the questions is provided in Appendix H. In this section, we state each question briefly and then summarize the responses from the merged documents.

# Q1: The quality and significance of the results of the Division's programmatic investments.

The consensus from the individual program reviews is that the Division is supporting science that is frequently transformative and impactful. In the discussion of Question 1, the two groups decided to focus on how one could develop more refined approaches for measuring significance and impact. Two main themes emerged:

### 1. How do you measure quality/significance?

The Q1 groups noted the primary emphasis on the Intellectual Merit of a given project, relative to the discussion of Broader Impacts. This disparate emphasis was noted in the review process as well and led to the comment that measuring "success" for Broader Impacts is a challenge for reviewers and PIs. The Q1 groups also wondered whether there should be increased emphasis on defining goals and metrics for PIs and CHE/NSF.

### 2. Are Annual/Final Reports structured usefully?

The Q1 groups discussed the annual reports for awards at some length. They noted that qualitative information was easier to extract from the annual reports than quantitative data (surprisingly), but that the former is considerably more time-consuming for PIs. They believe that post-award longitudinal analyses on the grant's impact on students and postdocs would be useful, but in large group conversations some reluctance was voiced about tasking PIs with this work. The groups noted that few PIs look forward to the annual report process. The annual report process attempts to be very general and all-encompassing making it very time consuming.

# Q2: The relationship between the portfolio and the Missions of the Division, the Directorate, and the Foundation.

The discussion of Q2 also had two major themes. One was the impact/interaction of the 10 Big Ideas on CHE, and other was how CHE interacts with the community in communicating new initiatives in the Division.

### 1. Foundation-wide initiatives and the 10 Big Ideas and Chemistry

The Q2 groups focused considerable energy here. The groups noted positively that the Division participated in several of the Big Ideas, but asked "How does the NSF define these initiatives and the 10 Big Ideas?", and "For whom have these initiatives been defined and prioritized?" The groups believe a stronger linkage to chemistry is needed for at least some new initiatives, and do not believe the current lack of linkage is in any way a negative reflection on CHE. The 10 Big Ideas feel "top down." The group also believes that, while new initiatives are desired and can be transformative, new funding needs to accompany them. New initiatives, tangential to the core mission of a Division, funded at the expense of critical basic science, are not a recipe for the health of CHE or any other Division.

### 2. CHE and new Initiatives.

The Q2 groups feel CHE is doing an admirable job here, particularly with its recent approaches. The CHE division has regularly held workshops and office hours focused on the larger initiatives to inform the community. Many of these have been moved online/virtual due to the recent COVID-19 pandemic. Attendance at these online sessions appears to be good. The committee felt that this strategy could be a cost-effective mechanism for informing the CHE community that should be continued. In addition to workshops, social media (e.g., Twitter, LinkedIn) could be helpful in promoting CHE participation in specialized opportunities.

### Q3: The Division's engagement in, and prioritization of, research initiatives.

The two Q3 groups focused on interaction of the Division with the community, ways to promote inclusion to the benefit of Foundation's mission, and echoed some themes about community access that Q2's groups surfaced.

### 1. Communication with the Chemistry Community

The Q3 groups believe that CHE does a good job of communicating with the larger community. There is a considerable amount of information that the community receives. The groups see the Division Newsletters as a strength, as are the regular emails that the Acting Division Director (Dr. Carol Bessel) provided during here time in the post. Some

noted that, while there was good information flow, they would have liked the information in a somewhat more streamlined form. Especially for young faculty the information can be overwhelming. Of course, we realize that there is always a fine line between "too much" and "too little" information and this may be a titration beyond the power of any finite group of chemists to accomplish. The groups appreciated the in-person sessions that occurred with some regularity at American Chemical Society meetings and other large gatherings of chemists.

# 2. Outreach to New PIs and PUIs and Institutions Educating Underserved Populations.

While the Q3 groups believe all three of the above populations require more attention, their primary suggestions focused on new PIs. Among their suggestions were: i) support mentoring efforts for new PIs (beyond the much-praised CHE CAREER Workshops), ii) perhaps increase the participation of junior faculty on panels. Item ii) was also suggested for PUI faculty.

### 3. Inclusion Initiatives

Greater inclusion supports the Foundation's mission and improves scientific outcomes. The groups discussed the Division's past involvement in COACh and OXIDE, and wondered when their successors would be developed. Is the Division no longer supporting such initiatives or have there been no proposals in these areas? Can the Division do more to promote new proposals in the area of inclusion? In addition, the groups wondered why COACh and OXIDE no longer receive support from CHE.

### 4. Virtual Presence Valued

The groups praised the Division's virtual office hours as a means to disseminate information about new programs and increase access. They also suggest that the Division increase its social media presence.

For a more complete presentation of the work of the three Portfolio Question Groups, see Appendix H.

### IV. Response of the Chemistry Division to the 2016 COV Report

Three recommendations were made by the 2016 COV. Assessment of the Chemistry Division's response to each recommendation is provided below.

**Recommendation #1:** Advocate additional funding for the Chemistry Division overall and maintain focus of existing funds on high-impact fundamental research. The percentages of funded proposals are low, and many strong proposals cannot be funded. Although the COV recognizes the challenges in the current funding climate, additional funds would greatly enhance the ability of the Division to maintain a strong research portfolio. The COV commends the Division for allocating a substantial portion of the budget to fundamental research and advises against diversion of existing funds from the core mission of fundamental research in efforts to initiate new programs. The highest priority should be funding the best fundamental science and transformative chemistry. In addition, the Division should ensure that the grant sizes are large enough to enable transformative chemistry with broad societal impact and should advocate for additional funds to increase both the number and the size of the grants.

The assessment by the 2020 COV is that CHE has done an excellent job of supporting highimpact fundamental research. This is true of every program the COV considered. However, as detailed above, the CHE budget was flat for the four years reviewed here (a factor almost entirely beyond the Division's control.) There were fluctuations in individual award sizes (increasing over time) but in discussions with the Division it appears this was due to a significant decline of collaborative proposals in 2018 and 2019, largely caused by the new solicitation by the Division that limited the number of PI submissions in a given year. Fewer collaborative proposals with large budgets allowed for larger Individual Investigator Awards but it is not clear that this is a positive tradeoff.

The Division does an excellent job of increasing its budget via co-funding opportunities; the net transfer of funds is positive and significant. However, these co-funds are modest compared to the needs outlined above.

Thus, the COV believes that the Division does an impressive job funding strong basic science with the budget it has. The overall budget has not grown, however.

**Recommendation #2: Enhance transparency of the reviewing and decision processes.** To maintain the trust and support of the chemistry community, the reviewing and decision processes must be transparent. Although the individual reviews and panel summaries are sent to the principal investigator (PI), the basis for the final decision is not always clear. The Program Officers write detailed summaries that synthesize the reviews and panel discussions and explain the basis for the final decision in the Review Analysis. However, the Program Officer Comments section sent to the PI is often very brief and less informative. Although the PI is encouraged to talk to the Program Officer by phone, these comments would be more useful if conveyed in writing. Thus, the COV recommends that the Program Officer Comments section contain more information about the decisions for declining proposals, including the allowable comments from the Review Analysis, consistently across the programs. The consistent and effective use of panels across the programs, supplemented by ad hoc reviews as needed to add specific reviewer expertise, is also recommended to ensure greater transparency of the reviewing process. In addition, the COV recommends that the Division better clarify the assessment, weighting, and accountability of the broader impacts to the PIs and reviewers.

In almost all respects this Division has done an excellent job responding to Recommendation 2. As detailed above the COV believes that decisions are made in clear and justified ways, that panel summaries, most panel reviews, and many ad hoc reviews provide considerable justification for their rankings, and that Program Officer Review Analyses are detailed, thoughtful and clear. It was generally felt that PO Comments to the PIs contained sufficient

detail and provide useful guidance. Some COV members, almost wistfully, wished that the RA could be provided to PI given its deep analysis. Perhaps a happy medium exists, but this was less a complaint about the PO Comments than a reflection of the general excellence of the RAs.

The only places where the 2020 COV finds little change compared to the 2016 COV assessment is the need for greater clarity with respect to Broader Impacts in the "assessment and weighting" of the BI, and the "accountability" of PIs and reviewers with respect to the BI. As detailed above, there was confusion in the COV about BI and "how much they count," "how are they assessed," and a perception that they are sometimes used capriciously to re-rank a proposal.

The challenge of disparate views of the BI may change as faculty who were "brought up" professionally in the CAREER Program mature, and more faculty are nurtured within its framework. To some extent there is a generational divide with respect to BI, but not exclusively. Superficial treatment of BI can still originate from young PIs, and profound commitments to BI are often displayed in the programs of senior faculty. However, the community would benefit from several workshops that clarify what is meant and what is not meant by BI and how they are considered in the review process. Community discussion may promote buy-in in ways that more documentation from NSF may never accomplish.

**Recommendation #3: Broaden the representation of proposals across types of institutions** and principal investigators. Inclusiveness at all levels is essential to the mission of the NSF. A wide range of perspectives and narratives provides the substance required to tackle global issues and to exert a significant impact. The COV encourages the Division to continue successful programs and create effective new approaches to increase the number of high-quality proposals submitted from different types of primarily undergraduate institutions (PUIs) and PhD granting institutions. The heterogeneity of institutions within the PUI and PhD communities is significant, and this heterogeneity should be recognized in the creation of solicitations and in the review processes that lead to the funding or declination of proposals. Moreover, the same attention should be given to increasing the number of proposals from underrepresented minorities (URMs) and women, while maintaining the expectation of approximately equivalent success rates across the various groups. Current approaches aimed at increasing the numbers of applications from URMs and women have not been fully successful, indicating that other mechanisms need to be created and launched.

As noted above, this issue continues to be a challenge for the Division. Several suggestions have already been made in this report regarding new approaches, but this is an issue not isolated to the Division.

### V. Program Review Reports

Each program review group noted in Appendix C was provided with a template that contained five sections. The first three sections address i) the quality of the review process, ii) the selection of reviewers, and iii) program management. Each program received detailed comments on these three areas. The fourth section addressed the program portfolio; the fifth section dealt with "Other Topics", and the COV Chairs decided to make these last two sections optional, since aspects of these questions were considered in later group discussions. In the following documentation we include the program review teams' responses to these last two sections if they were addressed. If they were not addressed we deleted the blank sections of the reviews, for the sake of brevity.

### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

### CAT: Chemical Catalysis

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Yes
Panels and ad hoc reviewers included experts and seemed well selected. All proposals were reviewed by least three reviewers by a combination of virtual panels and ad hoc mail reviews. The panel reviews were often supplemented with ad hoc reviews to reduce reviewer pressure, for needed subject matter expertise, and to give new reviewers some experience before panel participation. A majority of the submitted proposals were discussed at panel. This is encouraging, because panel reviews provide useful feedbacks that help not only the PIs but the experience as a panelist would help one to gain perspective on the latest development in the field.	
We recommend the use of panels unless there is a very clear reason for that not being the case. (Which was not quite the case in the e-jackets we reviewed). Panels also allow for the PO training in inclusivity to be used more effectively.	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Yes
a) In individual reviews?	

Some reviewers did not address the broader impacts as thoroughly as we would have liked.	
b) In panel summaries?	
c) In Program Officer review analyses?	
All merit review criteria were well addressed in the individual reviews, panel summaries, and PO review analyses.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	Yes
Most reviews were substantive. However, many were found to predominantly focus on the intellectual merit, with much less details given on the broader impacts of the proposal. Some reviews did not appear to offer sufficient commentary on the proposal itself, but rather, commented on the PI's record.	
Broader impact statements seem to have unequal weight depending on the productivity of the PI and seem, sometimes to be used arbitrarily (mainly to "kill" a proposal). We recognize that progress has been made in clarifying the meaning of "broader impact" there is more work that needs to be done to move towards a more uniform response to the proposed activities by the individual reviewers.	
The vast majority of reviews agrees with the letter rating (E, V, G, etc). However, there are a few reviews (less than 10%), where the letter rating given does not match the critiques. In less than 10% of the cases, the letter rating E was given with substantial critiques of the work. These cases were usually flagged and discussed in the Review Analysis.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	Mostly Yes
In nearly all cases, the panel summaries do provide the rationale for the panel consensus. However, the committee identified some cases in which the proposals were funded despite review ranking in the mid-range of the medium priority. While the discrepancy between the review scores was not addressed in the panel summary, it was found to be addressed by the program officers in the review analysis.	

The COV appreciated the template approach used in some panels and think that it resulted in a useful discussion. It is recommended that this template approach be used more consistently.	
Data Source: Jackets	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	YES
For the most part, PO review analysis provides a rationale for the award/decline decision, explaining clearly why and how the funding decision was made. The review analysis showed how the discussions in panels helped to converge towards a consensus.	
Various reasons and the thought processes were provided for the difficult decisions. One difficult decline decision noted that despite positive ratings, the proposal lacked enthusiasm by the panel, which was also seeking to broaden the portfolio of projects in the program.	
In one example, a low evaluation score was given in the review panel along with two stronger evaluations. The jacket provided the details about the review that indicate that despite the lower evaluation score, the comments were more in line with the stronger evaluations. Significant effort was made to rationalize the lack of consensus to arrive at an award/decline recommendation. In other proposals where consensus was not reached, the PO review summary provided the principal rationales each reviewer had in determining a proposal's score. However, one grant had fairly strong reviews, and while broader impacts regarding grant topic were strong, significant concerns were voiced throughout the panel with regard to limited impact from the particular grant.	
In a few cases, the conclusions regarding funding were not transparent. There was sometimes an apparent disagreement between the panel consensus and the PO recommendation. The information available in the eJackets was not enough to fully understand what had transpired. It seems that outcomes were not always defined by the reviewers' comments and panel enthusiasm, but by information not made clear in the e-jacket.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	Yes
PO comments to the PI were provided to explain why the decisions were made, but some PO comments were very short and not as detailed in the PO review analysis.	
For the proposals that were ranked highly but not funded, the clear communication to the PIs on the points for improvement would be highly helpful to the PIs. Additionally, information on the relative rank of the proposal, e.g., ranked 1 <sup>st</sup> in the medium priority, etc.) would be helpful for the PIs for improvement of the proposal. In these cases, the PI might benefit from a more detailed summary. In particular when the recommendations of the panel and reviewers does not seem to agree with the outcome, the extra effort from the PO will be valuable. <b>Data Source: Jackets</b>	
	Yes
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
The merit review process was utilized well for this program.	
There were two difficult decisions to fund that we reviewed out of the set in the Jackets. One proposal received a relatively low score, yet was still funded. In this case, there were comments by one reviewer that were found to be incorrect or inappropriate. Another proposal received lower ratings and was funded. This was a somewhat less controversial because, because although it was rated low, it did relatively well in the panel discussion (it was the top medium priority proposal).	
On the other side, several proposals out of the set had strong rating scores, yet were declined. One proposal scored high on its reviews, but was declined based on the comments from the reviewers that were not supportive. One other was declined with a high score, but it ranked relatively low in the panel, and it subsequently lacked preliminary data. Overall, these declines seemed like reasonable decisions.	
- <b>RUI</b> status: We would also like to note that it was very difficult for RUI proposals to be reviewed fairly in panels. We suggested they would do better by having only RUI proposals in one panel (not competing with R-1 institutions). But this is not feasible for several reasons according the CAT program officers. In some cases, panel members (from an R1 institution) are unaware of the demands on the time of the PUI investigator. This can best be managed by informing the panel members of the differences between RUI and regular grants, as is currently done. Within the CAT proposals we looked at, 4 had RUI status. Of these, 2 were reviewed by at least one panelist from a PUI. Two were reviewed by exclusively panelists from places other than PUIs. We encourage the program officers to strive for at least one panelist from a PUI on each panel	

that reviewers RUI proposals, or if that is not possible to request ad-hoc reviews.	
Comment on how the grant feedback could be improved.	
1. Generally, all review analyses were very constructive.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
The program officers and directors handled review process in an efficient manner. The discussion of the proposals shows that the reviewer expertise was sufficient and that the panels provided a great platform for sharing expertise. The use of ad-hoc reviewers in conjunction with a panel appeared to achieve the intended goal of adding depth to reviewer expertise in an area.	
We noticed the lack of industrial reviewers, which could be helpful in some cases. We also noticed the number of international reviewers and hope that these received enough context to evaluate broader impacts and proposals from less traditional institutions.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
Panelists having a conflict-of-interest with a specific proposal did not review that proposal and exited from the meeting during the discussion.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	
Something that should bear scrutiny with regard to CAT is the inclusion of women in panels and the roles that they serve therein. In the proposals given to the COV docket, review teams for each grant were only ~20% women. Many grants had no female reviewers in a primary, secondary, or tertiary role. In addition, the presence of a female reviewer as a primary was exceedingly rare (only 1 out of the funded grants and 1 out of the declined grants). An assessment of gender balance, as well as inclusivity of underrepresented groups, in grant reviewer roles is recommended. Beyond the funding rates for demographics, a balance in who has a voice in the recommendation of funding also demonstrates inclusivity.	

We encourage the chemistry division to analyze their reviewer pool for all types of diversity. PO should be supported in making their reviewer pool as diverse as possible.	
Perhaps it would be helpful to ask reviewers to suggest a few names of other qualified people to allow for a influx of new names that might not be obvious to the PO.	

# **III.** Questions concerning the management of the program under review. Please comment on the following:

### MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

Overall, the COV committee believes that the program is well managed. Many panels addressed a wide range of sub-topic areas and the proposals were reviewed in accordance with the two criteria of intellectual merit and broader impact. However, while both merit review criteria were considered in each review, there appears to be a lack of consistent assessment amongst proposals regarding broader impact. In some cases, the science alone and the training of the students on the project appear to be sufficient for broader impact; in others, outreach and educational initiatives appear to bolster this section. Some grants appear to acquire awards with generally weak or vague broader impacts. Some grants have outreach activities; some not at all. While it is important to allow some latitude to allow for PI strengths to be developed, greater consistency and assessment is needed. Greater oversight regarding execution of broader impacts is recommended (e.g., results from prior funding requiring broader impact assessment, annual report PO comments addressing status of broader impact execution)

We saw quite a variety on the styles of the PO comments. It would be nice to have a more consistent approach. We recognize that this a large division and that the amount of work for the PO is huge. We wonder how the work in CAT is divided and hope that the PO or POs are well supported. In particular, the broader impact area deserves attention at the division level to provide guidance to the individual PO officers (maybe even having dedicated staff).

The fraction of proposals by women and under-represented minorities in this program seems very small, and the trend is not promising. Even though the success rates are reasonable, this issue merits further review, which might include obtaining benchmarking data to compare with the broader community.

2. Responsiveness of the program to emerging research and education opportunities.

The program is responsive. The COV committee especially appreciated the funding of a grant with an industrial-academic partnership and the funding of a program for veterans and other innovative BI ideas. In terms of the emerging research areas, there are panels for confined spaces and heterogeneous surface catalysis, as the interest in 2D and porous materials begins to emerge. Focus on sustainable chemistry is also a plus.

However, the committee also believes that more information from the NSF on the current emerging research opportunities and NSF focuses would further help the PIs to submit applications to the programs that are best align with the research focus. Support for interactions with industry (student training) and community colleges (broader impacts) is appreciated.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

There were cases where the POs decided to fund or not fund specific topics based on portfolio balancing. The committee feels that a more transparent approach, by sharing with PIs (after proposal being rejected, or in some cases in advance), some information from the NSF perspectives on how the proposal could be considered funding, would be useful.

### 4. Responsiveness of program to previous COV comments and recommendations.

The program appears to be highly responsive to previous COV comments and recommendation. The feedback to the PIs has improved and the current program has placed more emphasis on heterogeneous catalysis with panels for confined spaces and heterogeneous surface catalysis to name a few. This should continue in the future.

Improvement in transparency of both the reviewing and decision process is also evident. This can still be further refined (see response to question 3 above). The inclusion of junior faculty from declined grants in proposal review and panels has the potential to address the poorer funding ratio of 1<sup>st</sup>-time investigator grants. An assessment of the success of this inclusion would be of great interest.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

### Balance across disciplines:

In general, the funding for heterogeneous catalysis is much less than that of homogenous catalysis in the CAT program.

### Projects that integrate research and education:

We commented that the criteria of Broader Impacts was not uniformly applied. Some projects had excellent BI and were funded, and others had less emphasis or more generic BI approaches and were funded. Likewise, the reviewers were not uniform in how much emphasis was placed on the BI criteria. Some reviewers were brief on evaluating BI, and others emphasized it much more.

### Award size and duration / Awards to new and early-career investigators:

The average award size appears to be reasonable with a significant fraction of the awards given to new PIs. Over 40% of proposals were submitted by new PIs in 2016-2018, but the number declined in 2019. In general, new PIs have lower success rates. Therefore, mechanisms to support them to be successful grant writing would be highly helpful. This may include: (1) proposal writing workshop and (2) webinar to prepare more junior PIs.

### Awards to different types of institutions:

The distribution of the awards to the different types of institutions looks appropriate. Most of the awards went to research-intensive PhD granting institutions, but the committee notes that this percentage fell in FY2019.

### Innovative/potentially transformative projects:

Based on PO review analysis, proposals had to be innovative or have a positive impact on the field to obtain funding. Expert reviewers from each respected field supported this viewpoint.

### Projects with elements of risk:

These is a good balance between funding the low-risk, low reward vs. high-risk, high reward research.

### Inter- and multi-disciplinary projects:

The program portfolio includes a good balance of inter- and multidisciplinary projects in partnership with other directorates. For the 4-year period, the number of awards where funds are flowing from other divisions/directorates to support CHE projects is roughly double the number of projects that are supported by CHE for projects primarily located in other divisions/directorates.

### **Projects that integrate research and education:**

The CAT program is more focused on research to support their mission. Education is encouraged d (for K-12 students, undergraduates, and graduates) but proposals will only be funded when the scientific merit is strong.

#### Participation of groups that are under-represented in science and engineering:

The funding rates for under-represented groups were in-line with the fraction of these groups in the discipline. The number of women and underrepresented minority involved in the funded programs have increase substantially in 2019 compared to 2016-2018.

#### Projects that are relevant to agency mission or National priorities:

Many proposals that were awarded focused on sustainability (SusChem), which is part of the program's mission. Funding for heterogenous catalysis appears to be much less than homogeneous catalysis. The COV noted that the balance of high risks and conservative work is appropriate. Portfolio could be improved by better integration of research and education, and a greater accountability to the "contribution to the greater society" is recommended, either via PO report approvals or in the prior results section of future submissions. It is commendable that industrial partnerships and student training via experience abroad included. An increase in multidisciplinary projects in the portfolio is recommended, assuming the COV docket profile is similar to the overall grants within CAT.

### **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

Involvement of women. Every single grant has female reviewers. We would like to know the compositions of the panel and presence of women in the panel and as reviewers.

In the catalysis section, the percentage of women involved appears to be in-line with the fraction of women in the discipline.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

More information on the NSF workshops, seminars, webinars on proposal writing to help preparing junior faculty members to write successful proposal.

- 3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.
- We compared the NSF and NIH funding and proposal review mechanism. There are several aspects of the review mechanism at NIH, which we would like NSF to consider.

Some of us have been PI on grants at both NSF and NIH. The NIH system of using the same reviewers every time (by established study sections) has some advantages. Many of us have all had the experience as grant writers of addressing an NSF reviewer concern and then in the next proposal cycle, the reviewers have a different set of critiques or concerns (and maybe they don't

care or don't know that you addressed concerns from another past reviewer). This could be solved a number of different ways:

- Have at least one reviewer that reviews both the original proposal and its revised version. This reviewer could be ad hoc, or a member of a panel.
- Have study sections or assemble the same panel two years in a row.
- If the above 2 suggestions are not logistically feasible or go against other NSF ideals, consider then a simple option of giving the PI one page in which they summarize the past reviews and briefly state how they addressed them. In the NIH system, this is called a one page "response to reviews". We already do this for journal articles that we revise.
- Furthermore, if NSF desires to do so, they can use this one-page response to reviews to potentially identify proposals that have not been responsive to past critiques. Potentially, the panel could choose to "not discuss" these proposals.
- We suggest that this could be first test run for the CAREER proposals. CAREER proposals that are resubmissions are an ideal test case because the PI only gets three opportunities to apply. However, in the long term the approach could be applied to other programs as well. The CAREER proposals could be labelled as either new (if the idea is fundamentally different than a prior submission and the proposal is at least 50% different from a prior submission) or it could be labelled a revision if its less than 50% revised. The number need not be 50% as the cutoff, but it could be whatever cutoff the program officers feel is sufficient.

The guidelines to reviewers regarding broader impacts might be improved by the addition of a request to describe scientific broader impacts separately from education/societal broader impacts.

It would be nice if the division was able to inspire a sense of community among its members. Perhaps a session in an ACS meeting where PI gave talks and officers were available would be useful in this regard.

4. Please provide comments on any other issues the COV feels are relevant.

There is always the issue of equity and fairness. The two proposals that were rated low but still funded were from well-established investigators from highly productive labs. Maybe the decision is warranted because these groups are very productive. But the issue is there nonetheless.

Perhaps PI can be encouraged to provide mentoring to scientists in institutions where there is no expertise to help them improve and refine their proposal or otherwise isolated. This could be facilitated by NSF and count a broader impact educational effort.

### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

### **CCI: Centers for Chemical Innovation**

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	YES
The merit review process for the CCI program is robust and multifaceted, which is appropriate for investments of this magnitude. Review procedures for Preliminary, Phase 1 and Phase 2 proposals are appropriate given the number of submissions for each. Short, preliminary proposals are assessed using panel reviews supplemented with ad-hoc reviews. Ad-hoc reviews are critical to the CCI program because by design, centers bring together investigators with vastly different areas of expertise together. The COV was impressed by the number of reviews for the preliminary proposals. Seven individual reviews as opposed to the standard three reviews was not uncommon for Phase 1 proposals. The program is to be commended for investing in this critical stage of proposal filtering and triage.	
The process of review for Phase I proposals begins in much the same way as preliminary awards. Several reviews commented on the collaborative nature of investigative teams and the ability of each proposed center to yield truly transformative research findings. Awarded Phase I proposals were reviewed by panels two years into the three-year lifetime of these grants. This midterm Panel review is an excellent way of assisting awardees prepare competitive Phase II proposals.	
Fifteen individual reviews for Phase II proposals was not uncommon. Panels were assembled to review projects. Phase II added site visits, including reverse site visits, to the Phase II review procedures. Considering that CCI visits typically take place at multiple institutions, the reverse site visit is an acceptable	

way to assess the overall quality of Phase II proposals. However, we urge the NSF to default to in-person site reviews rather than virtual whenever possible. These are crucial decisions wherein the interaction between the PI, faculty and students plays a critical role. Evaluation of these interactions is facilitated by observing how the team works together to address questions.	
Data Source: jackets	
4. Are both merit review criteria addressed Both intellectual merit and broader impact are addressed in individual reviews,	YES but unevenly
in panel summaries and in the Program Officer review analyses. Intellectual merit: All three: reviewers, panels, and POs, do an exceptional job evaluating the intellectual merit criteria. Program Officers in particular are able to ascertain constructive feedback from individual reviews and panel summaries necessary to make award recommendations. It was noted that in some cases panelists assigned low marks to a proposal, but had mostly good things to say about it. In these cases, the Program Officers were able to make award decisions on proposals that fell into the medium priority range. The reasons for decisions to over-ride a panel recommendation were well documented and valid, which speaks to the role of experienced, transparent and thoughtful leadership within the CCI program. It is clear that the CCI values innovative, transformative science.	
<b>Broader impact:</b> The science in itself can be broader impact. However, the COV would like to see more substantive feedback on the Broder Impact criteria, especially in individual and panel summary reviews. Typically, panelists and panels were able to comment on the impact of proposed outcomes on society. However, several were not as good as determining if plans for broadening participation and INCLUSION were appropriate and likely to be effective. Some proposals provided substantial detail on what their institutions were doing to broaden participation while proposing to do very little themselves. Lack of attention to broadening participation by funded proposals is a lost opportunity, especially for the CCI. The CCI <i>could</i> catalyze transformation of the research enterprise to be more reflective of the general population. Innovation is fueled by diversity in thought. Consequently, constructive feedback regarding broadening participation in the CCI is merited.	
Program officers did a good job providing feedback on the quality of broadening participation activities. However, our review of this portfolio showed that proposals that reviewed well with respects to broader impact, including broadening participation were less likely to be funded. This was especially true in the Phase II awards wherein plans on both criteria were developed more completely. The COV suggests that encouraging CCIs to include at least one institution recognized for research training above research productivity may help to broaden participation in CCI awards because these types of institutions often serve more diverse populations of students. With significant resources and time, CCIs should have the capacity to reach beyond the traditional sources for diverse participants	

<b>Data management:</b> Review of Data Management Plans could be improved. Because CCIs generate lots of data, the scientific community would benefit from a more robust plan for data sharing.	
Data Source: Jackets	

<ul> <li>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</li> <li>In most cases the quality of individual reviews is good providing useful feedback to the PIs and Program Officers. However as noted above, while substantive comments are universally provided for intellectual merit, less is provided for broader impact, and minimalistic feedback is provided for the Data Management</li> </ul>	YES focused on intellectual merit
Plan. Reviewer feedback varied from phase to phase. In Phase I, feedback was mainly confined to big picture issues. This is deemed as appropriate for this planning phase. The Phase I full proposal reviews included very detailed feedback with both phase I and phase II plans addressed.	
Due to the suspension of Phase I competitions, this COV was not provided with any Phase I to Phase II proposals.	
The Phase II renewal phase reviews included very detailed feedback from many reviews (~15). Given the substantial continuing investment, extensive reviews are considered appropriate.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	YES
<ul> <li>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</li> <li>The panel summaries were excellent. In cases where consensus was not achieved there was a detailed discussion of the reasons why, and the pros and cons of each opinion.</li> </ul>	YES
<ul> <li>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</li> <li>The panel summaries were excellent. In cases where consensus was not achieved there was a detailed discussion of the reasons why, and the pros and cons of each opinion.</li> <li>It is to be noted that the individual reviews were not always as useful as the panel summary, especially those generated for evaluating Preliminary and Phase I proposals. Individual reviews contained inconsistencies in content and depth. There were cases wherein individual reviewers did not follow the required template. There was discussion in the COV committee regarding the relative quality of individual ad-hoc reviews in comparison to those prepared by panelists.</li> </ul>	YES

Although the panel summaries were typically of high quality, panel prioritization (high, medium, low) was occasionally in disagreement with the Program Officer award recommendation. Program Officers produced comprehensive documentation of the rationale for award recommendations, especially when the decision disagrees with panel recommendations or priorities. When a decision went against the panel recommendation, the notes in the eJacket included additional information that the Program Officer used to make an award recommendation. The COV recognizes this as a strength of the program because it provides a mechanism for the program to address biases in the community towards, including technical and geographic area bias, that may be overlooked by the panel. <b>Data Source: Jackets</b>	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	YES
There was a detailed analysis. In phase I preliminary, there was often discussion of how to make a resubmission better, e.g. by providing a clearer or more comprehensive long-term picture. In phase I full, funded proposals reviewers provided directions for how to evolve.	
In the case where the program went in a different direction than the panel recommended, the decision was made with significant consultation with the broader NSF as well as other federal funding agencies. The basis of the decision is transparent and soundly based.	
The review analysis in this program stood out for the level of detail. Panel summaries were uniform in addressing all the points on the template; the summaries helped standardize the review process, especially when individual reviews did not conform to the template. The COV perceived most individual reviews as balanced except for the issues mentioned above when the reviewers declined to follow the template and did not address all aspects.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	YES
The CCI program is unusual in the Phase II renewal stage: proposals are competing only against their plans and expectations. For phase II renewal, the PO documentation was very extensive concerning the decision to renew or terminate the project. In the case of termination, reasonable funding was supplied to enable an orderly shutdown.	
The Phase II projects in CCI program are unique within the division in that the PO is actively involved in overall guidance of the project. This guidance	

necessarily means that there is ample communication between the PO and the PI. The PI is well informed. The COV recognizes that POs encouraged PIs to call them to discuss the pre- and proposal reviews, but particularly for declined proposals, the COV encourage more feedback from the POs to the investigators. Given the scope of the proposals to this program, the COV suggests that direct outreach from the PO to declined PIs would both increase transparency and strengthen any resubmissions.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	Mostly effective
The review process is fair and well-documented. The COV notes once again, that the CCI program is unique: this program needs to demonstrate results.	
The COV recognizes that this program takes risks. The reviewer(s) could be asked to specifically do a risk analysis. The COV found it difficult to judge how risky some proposals were, or if a plan is in place if something fails. The COV recognizes that the chemistry advances that result from the centers' research can themselves be transformative. However, the COV recognizes that the POs in this program need to balance the need for quantitative metrics (e.g., publications) vs. the qualitative contributions, such as training, networking and building new synergistic collaborations. While the broader impact on research is often gauged by publications in high-impact journals, the projects should produce results that alter the direction of the field and have an impact on the broader society. The COV suggests that project reports should include this aspect of the intellectual merit; it appears to be nearly lacking.	
Both the panels and reports stressed the importance of center connectivity, and this is clearly represented in decisions as about funding, and we see this in the annual reports. It is also clear in the Phase II that the centers have evolved significantly, as weak components are removed, and new investigators are strategically selected.	
The COV suggests that in this program, broader impacts should go beyond and be more creative than in single PI grants. Reports should indicate steps taken to impact broader representation on the faculty at the top research institutions.	
The COV was particularly concerned about the impact of the very significant investment of resources. There needs to be an opportunity to take a very high-level view of the program. This COV provided some comments within the posed questions; but there is a missing component. The COV was mostly asked if the procedures and POs are effective; for the most part the answer is yes. We feel that there should be a mechanism for a higher-level program review; this would include the CCI and how it fits into the larger mission.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
The COV found the choice of reviewers for the CCI proposals to be excellent. Reviewers included those that were particularly knowledgeable in the areas of research discussed. Reviewers were also selected that could address the ambitious requirements for outreach, interacting with K-12, undergraduates including those studying at Predominantly Minority Institutions, and the general public. In short, the reviewer cohorts had a range of appropriate expertise and perspectives as documented in the eJackets.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
There was little discussion of COI conflicts within the eJackets and therefore the COV assumed that COI were addressed and resolved prior to panel discussions. In instances when COI was mentioned, the COV found that COI was handled appropriately.	
Data Source: Jackets	
<ol> <li>Additional comments on reviewer selection: Program scope and management are much more important than in other programs; reviewers are less an issue.</li> </ol>	YES
The COV commends the CCI POs for bringing together a large number of quality reviewers for the CCI reviews, especially for the Phase I and Phase II proposals. Although there was diverse representation within the reviewer cohorts (e.g. R1, PUI, URM, gender) the COV observed that the POs could increase participation of reviewers drawn from non-academic organizations and from outside of the United States. This would be most useful for Round II. Gaining input from reviewers could provide valuable input regarding management of large projects evaluating their likelihood of success and broader impacts.	

**III.** Questions concerning the management of the program under review. Please comment on the following:

### MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

The COV commends CCI for management of a complex and diverse portfolio of highly competitive grants with a broad scope over a long timescale. This is accomplished through frequent communications with the CCI directors (noted as unique to the CCI program), reflecting the interest of CHE in the CCI's success. The COV also comments the CCI for agility in response to unexpected events and is commended for taking appropriate action to help guide centers and keep them on track.

The COV discussed whether CCI is evaluating whether the Centers are more than the sum of their parts and how they reconcile innovation vs productivity. Through discussions with CCI POs, the COV came to understand and was satisfied with the fact that the success of the CCI portfolio is gauged by measuring what is valued, not by valuing what is easy to measure (e.g. publication counts). The COV committee recommends to continue highlighting the impact and success of the programs that are funded. They also recommend to find ways to assess long-term impact of these centers, whether directly or indirectly, considering both the intellectual and broader impacts.

The COV noted that reverse site visits have both positive and negative effects on the review process. In RSVs, the research team has selected certain individuals to present. NSF staff may miss some perspectives from others on the grant proposal, leading to perhaps a superficial sense of how the center is functioning. It is also recognized that RSV are a good compromise for not having to visit sites which can be costly and logistically challenging.

2. Responsiveness of the program to emerging research and education opportunities.

The COV commends CCI for being resourceful in engaging with new technologies for research.

With larger resources and personnel, CCI could accomplish more than single investigator grants For example, CCIs could potentially engage questions like:

1) How to reach out to communities that either do not have the resources or interest to engage in science professions (aside from REU programs).

2) How can the pipeline be transformed to make the faculty at top ten institutions look more like the diversity of the general population?

With larger resources and personnel, CCI are also primed to quickly respond to emerging research. The COV has a sense that Phase II center are fulfilling aims however it is not clear how flexible they are in being able to change scope to respond to changes in their own results or emerging research.

The COV values that CCI POs have regular communications with the center directors, providing guidance to the teams, and encourage continuation of this practice.

In addition, the COV recommends exploring whether an external advisory board, or similar construct, may be beneficial for large grants to allow the CCI centers to easily change directions should it need to. Factors to consider may include: Would NSF be able to help set up such infrastructure? Would it also be valuable for the PI's to have mentors to help guide them? What role should the NSF provide in helping to guide the research to provide guidance but not dictate research? Would it benefit the CCIs to have an embedded NSF member that rotates though each of the CCI teams?

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The COV recommends expansion of topics that would be appropriate for CCIs. The emphasis has been on predominantly traditional chemistry content (e.g. Synthesis and characterization). The COV urges the program to broaden what is defined as chemistry, developing more forward-looking aspects of chemistry.

The COV commends CCI management for taking accountability of decisions on making awards. The decisions weren't always in agreement with reviewers and justifications were thoroughly documented and often based on risk review and willingness of the NSF to take risks toward innovation and potentially transformative research.

4. Responsiveness of program to previous COV comments and recommendations.

The majority of the 2016 COV comments regarding the CCI program were complimentary and therefore did not warrant a responsive action.

There was one critique reiterated by the 2016 COV from the 2013 COV: "We encourage the NSF to explore and develop positive interaction between CCI and other chemistry-containing centers in areas that are complementary. For example, integration and joint support of outreach and public educational efforts, a shared interest by all centers." The 2016 COV concurred suggesting that "Co-funding with other agencies may be possible" as a means to those ends. This COV also urges CCI to consider joint funding with other sections of NSF.

In addition, this COV acknowledges response of the CCI to the major recommendations from 2016 COV to CHE as a whole: expansion of the program and attention to transparency in decisions rationale to the PIs. The current COV feels that encouragement of partnerships with industry and RUI institutions is still warranted.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

CCIs tend to produce high impact results, including papers in top journals. Also, CCI's are very good at interdisciplinary collaborations. And in some cases, by bringing together researchers that might otherwise compete, this has fostered collaboration. However, because of their emphasis on joint publications, this tends to devalue individual accomplishments. There are some faculty who avoid CCI's, in part because of the gestation period, in part because of the management and outreach responsibilities, and in part because they prefer to do their own thing.

At this point, the CCIs have been in existence for long enough, it should now be possible to evaluate the nuggets that the centers have produced that have altered the direction of chemistry – results that are clearly attributable to the center as opposed to a collection of individual PIs. The COV suggests that there should be a comprehensive review of the program – not the same as the COV – but rather an emphasis on whether this mechanism is altering the course of the field.

### **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

The CCI management needs to be strategic with respect to ideas for CCIs that address important societal needs. CCI is a good mechanism to fund ideas that need long-term efforts.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

Especially for Phase II, the centers need to continuously reinvent themselves, reaching to ever more impactful results.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

Seek joint programs with other NSF divisions that allow for 50/50 CCI's.

4. Please provide comments on any other issues the COV feels are relevant.

Phase I currently requires a lot of effort for little funds. Particularly for the center director, funding is less than a single investigator award.

### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

### CLP: Chemistry of Life Processes

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Yes
Panels and ad hoc reviewers included experts and seemed well selected. COV was pleased to see that a large majority of the proposals were reviewed by panels. COV viewed the ability of the panels to rank proposals to be of high value. In-person panels offer the benefit of engaging the PO with the members and allows them to play more of a leadership role. In-person panels allow networking opportunities for young faculty, but virtual panels can increase participation by those who have very busy schedules. There is also an environmental benefit to virtual panels. COV therefore recommends a balance be found between in-person and virtual panel reviews. Mixed panels (half in-person, half digital presence) could be considered, but only if a critical mass of attendees can be onsite. COV is also concerned that virtual attendees in mixed panels will not have the same level of participation. The Low, Medium, and High Priority ranking system is a good way to sort proposals rapidly and clearly. COV recommends that, as much as possible, panelists be given a rough idea of how many proposals can be funded in a given group.	
2. Are both merit review criteria addressed	No
a) In individual reviews?	
Both criteria are adequately addressed in the large majority of the individual reviews. However, COV notes that the Broader Impacts were less emphasized	

by some reviewers in CLP than by other reviewers. Reviewers should instructed to address both criteria in details. A recommendation would have more structured quidance/feedback for review submission	ld be Ild be to
b) In panel summaries?	
Yes. In panel reviews both criteria are considered.	
c) In Program Officer review analyses?	
Yes. The COV committee commends the PO for writing very thoroug and meshing all the reviewers' comments.	gh analysis
Data Source: Jackets	

es
es
5. Does the documentation in the jacket provide the rationale for the award/decline decision?
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The COV team commends the program officers for writing Review Analyses that are very thorough and clearly explain the bases for decisions. These summaries showed how the discussions in panels helped to converge towards a consensus. The vast majority of cases were well-explained in terms of the review criteria and other factors. However, in some instances, there were borderline cases in which the decision didn't seem justified with respect to the panel summary and individual reviews. There were differences of opinion within the committee about whether additional rationale is needed for decision on borderline cases. <b>Data Source: Jackets</b>

<ul> <li>6. Does the documentation to the PI provide the rationale for the award/decline decision?</li> <li>COV notes that the POs have made significant efforts to add transparency in their decision process, to the extent that is possible. This was a recommendation of the previous COV review. COV realized that some decisions are based on sensitive decision criteria that cannot be shared. Some of the contents in the PO Review Analysis would be valuable to the PI and could be included in the PO comment.</li> <li>Data Source: Jackets</li> </ul>	Yes
<ul> <li>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</li> <li>On borderline cases, The POs made sure that the decision was properly rationalized to the PI, but it might be necessary to provide additional details.</li> <li>COV would like to note that it is very difficult for RUI proposals to be reviewed fairly in panels. COV is concerned that there could be unfair comparisons of proposals from PUI investigators with proposals from R-1 institutions. COV notes the importance of explaining that PUI investigators 1) have a heavier teaching load and 2) lack graduate students to assist in mentoring undergrads. COV therefore recommends that panelists and the POs be reminded to weigh Broader Impacts more heavily when evaluating proposals from PUIs all had at least one PUI reviewer. However, often the panels reviewing RUI proposals included only 1-2 people from PUIs overall.</li> </ul>	
COV commends the PO's for supporting creative Broader Impacts activities, and for considering work-life balance in some funding decisions.	

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES with comments
The COV team commends the program officers and directors for handling the complicated reviewing process in an efficient manner. The discussions of the proposals showed that the reviewer expertise was generally appropriate and that the panel mechanism provided opportunities for sharing their expertise. However, as noted above, the addition of more ad hoc reviews would be beneficial for lending expertise in specific areas.	
Nonetheless, the COV team noticed that there was a lack of diversity (i.e. gender, race and institutions) amongst the reviewers. This doesn't allow the applications to be viewed from various perspectives, and can potentially decrease enthusiasm from a worthwhile proposal. Less diverse reviewers can lead to misunderstandings and can expose PIs to potential biases. COV recommends additional unconscious bias training of reviewers to insure a fair review process.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
Apparently yes, but it was difficult to judge based on the provided information. The 2016 COV committee recognizes that the "List of Suggested Reviewers and Reviewers Not to Include" was underutilized and this observation still stands.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	
The COV noticed that there is a lack of reviewers from foreign countries, industry or non-academic research institute that would expand the expertise.	
COV also noted improvement in the inclusion of PUI reviewers and recommends to continue this trendparticularly for proposals from PUI institutions (perhaps by adding more ad-hoc PUI reviewers). Thus, we suggest that POs educate the	

reviewers to have a good sense that excellent research is possible at any institution in the US. In essence, the POs need to make the reviewers aware of the cultural biases we have about what type of students and what types of institutions can produce good chemical research and train great future scientists. They should also instruct reviewers to consider the Broader Impacts to underrepresented communities more strongly, and to include panelists who recognize these benefits.	
COV noted a very low response rate to questions about Reviewer demographics in the materials provided for analysis. The COV committee highly recommends the NSF to instruct reviewers on the benefits of disclosing their demographic information to further the CLP mission towards diversity and fairness.	

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

Management is appropriate. The POs are doing an excellent job of managing the review process and organizing face-to-face panels as well as an appropriate job of selecting reviewers.

2. Responsiveness of the program to emerging research and education opportunities.

Not enough information was provided to assess this section fully. That said, the program seems to have funded some exciting new developments and they have also recognized when the Broader Impacts are outstanding.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The program did a good job of recognizing excellent science. This has led to good results and high impact papers for those PIs funded a few years ago (and for which reports have been filed and enough time has passed to evaluate papers). More clarity on the prioritization criteria would be beneficial--especially for the borderline cases.

4. Responsiveness of program to previous COV comments and recommendations.

The COV acknowledges that the NSF is working on the previous COV recommendations. However, there are still concerns regarding the Broader Impacts, as mentioned previously. The CLP should continue working on increasing the transparency of the decision process.

Potential recommendations regarding broadening the participation in URM PIs and individuals from PUI institutions:

- 1. URMs and faculty from PUIs are generally overloaded with service. This should be recognized and appreciated when evaluating the proposed scope of work and the results from previous NSF support.
- 2. The host institutions may not have the necessary in-house infrastructure for proper guidance. COV recommends the implementation of virtual training sessions that teach about proper grant management.

- 3. Paid Mentoring: The previous 2016 recommendation was to have URM identify a senior person to mentor the PI. The downside to this is that from one institution to the next, the PI won't necessarily have a good representative. It would be more beneficial to the PI to identify a senior person in their field for this purpose. The advantage is that the senior person would know the science. They could be invited out for a few days annually to see and evaluate the PI's lab interactions etc. They could provide feedback for grants and publications. The COV recommendation is that this mentoring comes with a stipend that is built into the grant so that the mentor has an invested interest to give their time.
- 4. There is a shortage of URM reviewers. URM PIs could be presented with additional opportunities to serve on at least one panel or as an ad hoc reviewer. This would be beneficial to both the NSF and the PI, and it would help to increase the diversity of the panels.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

The CLP program has received a total of 867 proposals over the last four years and the funding rate was consistent with other programs in the Division. The COV committee noticed an increase in the numbers of CLP awards between 2016 and 2019.

#### **OTHER TOPICS**

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

It seemed appropriate.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

COV members have been PIs at both NSF and NIH. We feel that the NIH system has some benefits, although it can take young investigators longer to receive their first NIH funding. The NIH system of using the same reviewers every time (by established study sections) has some advantages. We have all had the experience as grant writers of addressing an NSF reviewer concern and then in the next proposal cycle, the reviewers have a different set of critiques or concerns (and maybe they don't care or don't know that you addressed concerns from another past reviewer). This could be solved a number of different ways:

- a. Have at least one reviewer that reviews both the original proposal and its revised version. This reviewer could be ad hoc, or a member of a panel.
- b. Have study sections or assemble the same panel two years in a row.
- c. If the above 2 suggestions are not logistically feasible or go against other NSF ideals, consider then a simple option of giving the PI one page in which they summarize the past reviews and briefly state how they addressed them. In the NIH system, this is called a one page "response to reviews". We also do this for journal articles that we revise.
- d. Furthermore, if NSF desires to do so, they can use this one page response to reviews to potentially identify proposals that have not been responsive to past critiques. Potentially, the panel could choose to "not discuss" these proposals.
- 4. Please provide comments on any other issues the COV feels are relevant.

There is always the issue of equity and fairness. The vast majority of difficult decisions were ones COV felt were appropriate (Low rated proposals with MRR 3.5-3.75 that were funded and similarly high rated proposals MRR 4.1 that were not funded).

#### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

#### **CMI: Chemical Measurement and Imaging**

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Yes
Reviews were mostly conducted by panels with ad hoc subject area experts. Panel comments were typically more substantive and likely helpful to the Program Officer and PI.	
The RAPID and EAGER reviews provided to the COV, which contained reviews from NSF staff, rather than panel or ad hoc reviewers, were excellent. The reviewers provided detailed feedback on the proposal.	
Data Source: Information provided by Program and Jackets	
2. Are both merit review criteria addressed	Yes
a) In individual reviews?	
b) In panel summaries?	
c) In Program Officer review analyses?	
It is clear from the individual and panel reviews that both merit review criteria are addressed. The RA also includes both criteria.	
a) In most cases. However, the individual reviews were often brief in terms of feedback for the broader impacts criterion.	
b) In most cases. The panel summaries did an excellent job of distilling the feedback.	

c) Definitely.	
Data Source: Jackets	

<ul> <li>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</li> <li>Some of the individual reviewers provided very little substance. However, the panels served to balance those reviews by providing additional substance and dampening the effects of the outliers.</li> <li>Data Source: Jackets</li> </ul>	Generally, Yes but not always
<ul> <li>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</li> <li>Yes, however, many of the proposals we reviewed in eJacket ended up ranked medium priority, so it was difficult to judge how effective the consensus process was.</li> <li>The panel summaries help to further explain the individual viewpoints in the written reviews. The RAs are very thorough in capturing the consensus of the panel during the discussions.</li> <li>Many reviewers are becoming more comfortable and effective in virtual formats however, there are some advantages for in-person panel discussions.</li> </ul>	
Data Source: Jackets	YES
<ul> <li>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</li> <li>The review analysis would benefit from adding the ranking of each proposal with respect to all other proposals in each panel as other programs (ie. MRI) do. The program officer notes are very detailed and thoroughly describe the process, but the scores may be augmented by ranking, since the data is available for the review analysis. Providing the ranking on the panel would help to normalize the proposals across different panels when comparing funding decisions (award/decline). A score (E, V/G, G) may differ across panels but the ranking of the proposals in each panel provides some additional rational (documentation) to the PIs and to others wanting to assess the rationale for an award or decline decision.</li> <li>Many proposals ended up ranked medium priority and the program officer had</li> </ul>	YES
to make the final decision. In addition, in more than one case, the program officer overruled the panel. In all cases, reasonable justification was provided.	

We also noted instances of communications with other program officers in order to facilitate information exchange between programs.

## Data Source: Jackets

6. Does the documentation to the PI provide the rationale for the award/decline decision?	YES
The RA provides a summary to the PI but, in some (few) examples, the written reviews were of high quality but yet details for the declination of the proposal were not provided in the proposal summary or in the RA. In one case, there were no substantive weaknesses expressed in the panel summary and yet, the proposal was declined. There was also no constructive criticism in that one case.	
The Program Officer did an excellent job of providing feedback and including notes in the file relevant to the decisions. In all cases, the comments included direction to carefully consider the reviewer comments.	
In several cases, we noted additional phone calls and/or email communications with the PIs. These are incredibly valuable. Program Officers should consider adding an offer to talk to PIs (especially new PIs) whose proposals have been declined.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
Providing relative rankings across the panels and for each panel would assist in comparing quality and effectiveness. The use of virtual panels appears to be effective in standardizing the review of proposals in different panels over different years.	
It is not clear if a discussion on unconscious bias, inherent bias, etc. are introduced into the initial instructions of the written reviews or the panel review session. The practice of withholding other reviews until a reviewer has submitted her/his own review is a good way to reduce any bias, for example.	
The merit review process was generally of high quality. The ad hoc reviews were interesting and provided necessary subject area expertise, but the panel reviews often led to more substantive constructive feedback to the PL.	

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
In general, the reviewers appear to be very knowledgeable about the proposals being reviewed.	
Some areas of research within the CMI program are quite small and the conflicts of interest were fairly substantial as a percentage of the number of researchers in the field. In one case, we noted that the choice of reviewers could have been better; however, the Program Officer explained that reasonable choices were made given the way the PI had framed the work.	
Data Source: Program and Jackets	
<ul><li>2. Did the program recognize and resolve conflicts of interest when appropriate?</li><li>The program did a very good job of identifying and resolving conflicts.</li><li>Data Source: Jackets</li></ul>	YES
3. Additional comments on reviewer selection:	
Reviewers and panels were composed by a balanced cross-section representing different subject matter areas within analytical chemistry, a good representation from PUI and PhD-granting and also good diversity in gender and underrepresented minorities in reviewers and panel members.	
It also appears that a fair amount of effort was placed in recruiting early-stage researchers to serve as reviewers and to serve as panels.	
It would be worthwhile for the program to consider expanding the reviewer set for proposals in constrained sub-fields.	

## MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

CMI has significantly benefitted from seeking co-funding opportunities within NSF and even outside NSF. In one example, a proposal within CMI that would benefit from several applications sought and received co-funding from an agency outside NSF. It was also noted that a substantial amount of funds for CMI awards were leveraged from outside MPS, but within other NSF Directorates. The award/decline rate is approximately the same as other programs within the Division. New investigators were awarded at approximately the same rate as more established investigators.

It was noted that women and URM applicants were awarded at slightly lower rates than the balance of the awards especially in 2016 for women and 2018 for URMs. It was also noted that the number of 2019 proposals submitted was significantly lower than in the previous 3 years.

Evidence that the CMI program treats early and mid-career applicants fairly and no evidence to the contrary was found within the jackets.

There was a clear separation among measurement modalities with a clear division of funding that did not appear to unduly favor any one area. There was a noticeable effort to maintain a fair distribution of resources.

2. Responsiveness of the program to emerging research and education opportunities.

A fair number (~ 25%) of the proposals submitted to CMI were in specific initiatives such as computational and data-enabled science and engineering, SUSCHEM and in other emerging areas designated by NSF.

The responsiveness was good. One RAPID review was convened so proposal was reviewed in a timely manner. We also noted the inclusion of GOALI and RUI proposals in the portfolio.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The number of proposals awarded between 2016-2019 in the CMI program represents a balanced portfolio between the different analytical and imaging sciences assigned to the CMI program. The program also balances established areas of inquiry with emerging areas (see above) that are well represented in the jackets and also in the information provided by the program.

4. Responsiveness of program to previous COV comments and recommendations.

In the 2016 COV review, inconsistency in the review format (panel vs. ad hoc) was noted on a yearto-year basis. The review format for proposals evaluated in this COV was more consistent and appears to be in line with what one would expect for the type of proposals reviewed. Most standard proposals received a panel review (mostly virtual) with on average 3.9 reviews total, 2.8 from panel participants and 1.0 as ad hoc, exceptions being noted for RAPID and EAGER proposals. Notably in 2019, reviews were highly consistent with all proposals receiving 4 reviews in panel format, with 1 of those 4 reviews contributed from an ad hoc reviewer. CAREER proposals sometimes had higher numbers of reviewers, in line with the diversity in panel subject matter, which skewed some years slightly based on the relative percentage of CAREER proposals to standard proposals.

In response to comments in the 2016 COV report, additional information was requested on CAREER proposals funding rates, and upon evaluation, the trends appear to be an improvement over previous years.

In 2016 the COV review commented on the proposal scoring system in variances between different panels. In 2020, these variances remain however, there are some advantages for flexibility in the prioritization of proposals taking into account external factors in award decisions.

Evidence of constructive criticism throughout the jackets provided reinforce the priority given to provide this information to PIs when a decline decision is made.

In 2016, a request for a standardized review analysis (RA) was made. In 2020, a standard analysis was evident for each program officer within the CMI program.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

## **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

No gaps were identified.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

The program does a good job of balancing traditional measurement science with emerging and high-risk endeavors. The program is successful at co-funding because of the cross-cutting nature of measurement and imaging across the sciences.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

The data management plans are not given a high enough priority in the reviews. This may be a missed opportunity especially in light in the evolving importance in data sciences.

4. Please provide comments on any other issues the COV feels are relevant.

No comment.

5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

A summary analysis of outcomes (impact and productivity) resulting from awarded proposals (number of participating students, presentations, publications, highlights, etc.) would have been useful to the COV to assess impact and productivity. The data should be available to NSF from the annual reports and the COV members can, indeed, search within the annual reports but this is somewhat cumbersome and time-consuming. If there was a more accessible repository of the outcome data, this would facilitate the COV in future years.

#### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

## CSDM-A: Chemical Structures, Dynamics and Mechanisms - A

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

#### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Generally Yes.
Usually, a CHE research proposal undergoes a three-step process of review before a decision is made. The first step is several ad hoc (generally by mail) reviews. This is followed by a panel discussion of the proposal along with other proposals in that area. Finally, the relevant Program Officers (POs) reviews the proposal and the other input and makes a recommendation. This recommendation generally amounts to the final decision, as the POs are justifiably given a large role in making such decisions. Overall this is a process that is fair and consistent resulting in excellent research and educational efforts. Consistent and effective use of panels across the programs, supplemented by <i>ad hoc</i> reviews as needed to add specific reviewer expertise, is encouraged to continue to maximize equity and transparency of the reviewing process. The combination of reviews and panel summaries enables critical advice and helpful insights to be shared with the principal investigators (PIs) as a result of the reviewers who may be unable to travel to an in-person panel, which can help to achieve appropriate expertise and diversity in panel reviews. It is important, however, that POs have the option to conduct ad hoc review, when necessary, in order to provide the most comprehensive review of proposals.	In some more data may be needed.
cases where a specific institutional reviewer was needed (PUI, UMIs, etc.) the failure to return a review could have larger impact on the decision. From 2016- 2019 there is a 35 percent rate of decline. Late reviews were also at the ten percent decline rate.	

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A mechanism for coaching reviewers, or development of a feedback mechanism to reviewers, on best practices might improve the review system.	
This would need to be done in a manner that does not interfere with reviewer	
confidentiality. NSF should ensure that a program officer includes	
considerations for determining whether a reviewer is currently overly subscribed	
(to complement the electronic system used by NSF reviewer assignments).	
The POs play a crucial role in overseeing the review process and selecting reviewers with appropriate scientific expertise, while maintaining diverse representation from reviewers at different career stages and of both genders. Efforts should continue to identify competent reviewers and to increase the participation of underrepresented minorities whenever possible. Program managers play a very important role in making sure that less common perspectives are heard by the entire panel.	
There were questions on the relative influence that ad-hoc and panel reviewers have on proposal decision. Results from previous support are important, but reviewers must remember that they are reviewing the proposal rather than the investigator.	
It is difficult to see whether the diversity of reviewer participation matches that of diversity of faculty. The program has done a good job at reaching out to a wide range of reviewers from many subdisciplines and geographical locations. A greater level of inclusion should be a continued goal.	
Other questions that some COV members have include: What is the reviewer declination rate in panel vs. ad hoc reviews? Are there mechanisms for mitigating declination rates? Is virtual panel review a good substitute for onsite panel reviews? How does the PO weigh whether a comment is a suggestion or critique?	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Generally, YES.
a) In individual reviews?	
The choices of ad hoc reviewers is adequate. The reviewers were clearly experts in their fields and represented the variety of experience that is needed to provide an overall balanced assessment. In some cases, broader impacts for individual reviewers were not well addressed.	
b) In panel summaries?	
Panel reviews are in many ways complementary to the ad hoc reviews. The	
panel reviews use as important input the ad hoc reviews that have been	
provided, but the panelists also make their own judgments and, most	
The panel reviews provided very useful perspectives to the POs.	
c) In Program Officer review analyses?	

In general, the panel was impressed with the thoughtfulness of the proposal evaluation summaries and recommendations provided by the POs. Although well informed by the <i>ad hoc</i> and panel reviews, the POs were not reluctant to depend on their own expertise and experience. Efforts should continue to identify competent reviewers and to increase the participation of underrepresented minorities whenever possible. Attention to both merit review criteria were viewed as critical.	
Reviewers and POs need to be mindful to avoid over-use of Broader Impacts and data-management plans to make decisions that could be construed as arbitrary. Reviewers need more guidance on what defines broader impacts. Pls need more guidance on how the Broader Impacts of proposed activities are evaluated and used in funding decisions. In addition, the uniqueness of the proposed Broader Impacts activities should be specific to the PI, not just the institution. <b>Data Source: Jackets</b>	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals? In general, reviewer commentary was good, but there were examples where this was not the case. Program officer analysis was generally thoughtful and responsive to reviewer commentary. Some attention would be worth considering to whether or not proposals with only three reviews had appropriate and substantive reviews. This appears to be the case, but not all eJackets had substantive notes. Adequate reviews are provided in the majority of cases, but uneven and insufficient levels of comment are made by reviewers in some cases. Panel review and review analysis corrected much of this concern. However, it would be important for the process to encourage more effective comments by reviewers, which would be very helpful to the POs. Data Source: Jackets	YES
<ul> <li>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</li> <li>Yes, panel summaries were well done and provided balanced perspective on reviewers' input. The panel reviews provided very useful perspectives to the POs.</li> <li>Data Source: Jackets</li> </ul>	YES

5. Does the documentation in the jacket provide the rationale for the award/decline decision?	Yes
In general, the panel was impressed with the thoughtfulness of the proposal evaluation summaries and recommendations provided by the POs. Although well informed by the ad hoc and panel reviews, the POs were not reluctant to depend on their own expertise and experience.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	Yes
An important part of the review process consists of providing feedback to PIs following the funding decision. Such feedback is critical to ensure that the process is fair and transparent. It also has an important role in educating and supporting scientists so that, especially in the case of a declination, their next proposal submission may be more successful. The review analysis and program officer comments to the PI were consistent and provided sufficient information to the PI to understand the basis of the PO's decision. The review analysis is well developed to support the PI in next submissions if proposals is declined. PO provided especially well developed responses to the declined CAREER awards.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	YES
Significant progress has been made to increase clarity about the relevance and expectation of the Broader Impacts. However, it seems that sometimes the BIs are used in ambiguous ways to either support or decline a proposal. A more transparent, equitable, and more quantitative rating system seems to be required to evaluate the Broader Impacts across multiple proposal.	
For PUI and under-resourced institutions and new PIs, it would be useful for mentorship of researchers in such groups. Outreach, similar to early-career workshops, that reach into non-PhD granting institutions would help researchers in this class. Mentorship should concentrate on both proposal technical development of ideas and proposal writing.	
See comments about selection of reviewers below	

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	Yes
The POs do an excellent work selecting qualified reviewers. The program generally had a sufficient number of reviewers with appropriate expertise and qualifications for obtaining good advice. The program sought expertise from a large number of reviewers and seldom used expertise of the same reviewer more than once.	
Selection of reviewers was discussed in detail. Overall panelists thought that the review process could be significantly improved if reviewers were asked to review less often. Reviews with too little detail are not useful to the PIs or the funding decision. Competent reviews are sufficiently detailed to be useful to the PI and the funding decision. More substantial reviews are appropriate to evaluating the appropriateness/competency of the reviewer.	
Reviewers: Consider 4-year grants to reduce grant writing time: "less renewing, more reviewing" (see comment above about being asked to review less frequently). The size of the awards could always be larger and the duration of the award could be lengthened. This is probably already being done, but flag new faculty to serve on panels where expertise is appropriate. Panels should avoid more than one novice reviewer.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	Yes
Based on reviewer selection it appears that the program carefully screened the reviewer pool and successfully avoided choosing reviewers with conflicts. The ejackets did include a few notes about COI resolution.	
Data Source: Jackets	
3. Additional comments on reviewer selection: (See above)	
Increasing the diversity of both women and URMs should continue to be a priority and a focus of the POs to enhance a wide range of perspectives and	

discussions among the panels and ad noc	reviews. This may mitigate any
inherent and unrecognized biases within th	e review process. Specifically, it may
be valuable to identify inherent biases in re	viewer demographics with respect to
PI demographics. Giving early-career facul	ty a chance to become reviewers (ad
hoc or panel) will provide those faculty with	h important information about the
proposal writing and submission process.	

## MANAGEMENT OF THE PROGRAM UNDER REVIEW

#### 1. Management of the program.

There was a strong consensus that the program is well managed and that decisions are generally made with good rationale. The program officers are commended an excellent job. The program officer provides sound justification for funding decisions that is tied to the review data. The Review Analyses are well done to explain the decisions about funding.

There were several comments on new investigators and RUI proposals. Among the eJackets provided for review, there were no RUI or CAREER awards (only declinations). Unfortunately, the COV team assigned to review the program did not request to see more information. Nevertheless, support for young investigators is encouraged as necessary to the long-term viability of the program. It is noted that the funding rate for new PIs is low but has improving over the over the last four years. There is still a need for further improvement in funding rate for new PIs. Impact of once per year submission on young researchers is negative. There could be better advertisement of proposal preparation workshops. This was mentioned in the earlier COV reports. NSF could send advertisements to all department chairs once a year to make sure that assistant professors are aware of these opportunities.

#### 2. Responsiveness of the program to emerging research and education opportunities.

It was observed that the program manager took measures to work with potential PIs from less traditional institutions such as four-year colleges. The program manager spends a lot of time talking with PIs and coaching declines and strongly encourages PIs to think about core physical chemistry rationale. This is especially important for early-career scientists that need to remember to base their proposal on pure science. The CSDM-A portfolio is diverse, but further strengthening may be achieved by further diversification in novel areas of physical chemistry. For example, some programs are growing, and perhaps moving physical chemistry intensive proposals to CSDM-A would be of use.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

Awards are well aligned with supporting the interface between experimental and theory.

4. Responsiveness of program to previous COV comments and recommendations.

No substantial concerns are found. Earlier comments about refining the broader impact of this program have been taken seriously. Program officers have clearly addressed the previous COV guidance regarding comments to the PI reflecting the review analysis. Two notes are: (1) no specific reply from CSDM-a to the comments in the COV 2016 and (2) some questions about the quality and quantity of reviewers remain.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

#### **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

There is a general need for rejuvenation of the physical chemistry field.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

What are your program specific goals?

The program is focused on traditional physical chemistry and on using these techniques to advance the overall mission of NSF. Strong overlap with computational chemistry.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

The program included a good mix of award with program reference codes that address mission areas of the National Science Foundation. Almost all of the awards are linked to one or more reference codes that are linked to the NSF mission areas. For example, there are 18 in the area of clean energy, 2 in hydrogen storage, extremely strong overlap with computational science and engineering, 16 in quantum leap, three in quantum information science, and 36 in unsolicited nanoscience.

a. Please provide comments on any other issues the COV feels are relevant.

It is very important for program officers to travel to national meetings under ordinary circumstances. Being able to reach out to HBCUs and minority-serving colleges would provide a means for enhancing the proposal pressure from these institutions. Providing academic-year support to minority-serving institutions is an important need given their teaching loads and additional collaboration between educational and human-resources parts of NSF and physical sciences should continue.

b. NSF would appreciate your comments on how to improve the COV review process, format and report template.

COV members would appreciate information that allows better review of an entire panel. Perhaps data for two years rather than four would facilitate review of the panel. Access to more data about the individual reviewers would better parse the activities of the panels. More information about the reviewers would be useful to COV; this includes whether reviewers have reviewed previously, if the reviewers average ranking is norm or above or below average, and if reviewers has been funded by NSF / is currently funded by NSF.

An assessment of the reviewer pool may be of use to NSF. Similar to the statistical assessment already performed on PI demographics, undertake a statistical assessment of the reviewer demographics. With the data, query whether there are inherent biases in the reviews of one demographic with another PI demographic.

#### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

#### CSDM-B: Chemical Structures, Dynamics and Mechanisms - B

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

## I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate? The review of CSDM-B proposals for 2016 - 2019 was predominantly by review panels. There were seven separate review panels, distinguished by their different sub-disciplines. Some of the reviews of proposals in these panels were supplemented by mail-in reviews. The COV is of the opinion that panel reviews provide the most effective and fair evaluation of proposals. Discussion within panels helps to resolve differences in individual reviews. In addition, the Panel Summaries are typically very helpful for PIs in considering the basis for an award decision. The use of high, medium, and low priority rankings to categorize proposals in panels seems appropriate and fair. Not discussing lower ranked proposals, but allowing panelists to "call back" these proposals for discussion, is an efficient use of panelists' limited time. However, in these cases, it must be clear to the Program Officer that the provided reviews contain sufficient justification for the low ranking, especially as these proposals do not receive a Panel Summary. As none of the proposals considered including site visits, this method was not discussed.	Yes
CAREER program review often needs ad hoc to supplement panel reviews due to breadth of expertise needed.	
Given the breadth of the CSDM-B program, not all proposals fall into the review panel sub-disciplines. These proposals (ca. 15% of the total considered) were reviewed exclusively by a mail-in process, with the Program Officer making a funding decision based on these reviews. While there are advantages to mail-in	

reviews, including the larger number of potential reviewers that can be enlisted, the review of these proposals lack panel discussions, which are typically an important component of the review process. In cases of mail-in only reviews, it is important that the PI receives detailed PO comments.	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Yes
a) In individual reviews?	
b) In panel summaries?	
c) In Program Officer review analyses?	
Individual reviews almost always provide strong feedback on the intellectual merits of the proposal. While the evaluation of broader impacts is more subjective, the Panel Summaries typically provide fair and reasonable evaluations of broader impacts, although the broader impacts section can sometimes be very brief. The COV felt the Program Officers' Review Analysis reports were outstanding and provided clear summaries of reviewer comments and justification for funding decisions. The review process has sought to increase clarity regarding the evaluation of broader impacts. The current online system for collecting reviews requires reviewers to address both categories. In addition, the lists provided by NSF of activities that constitute broader impacts is helpful for both PIs and reviewers.	
In the individual reviews, the emphasis on intellectual merit is far greater than that of the broader impacts. Broader impacts are more subject to interpretation and context ( <i>i.e.</i> , type of institution of the PI and reviewers) than the intellectual merits. For an individual reviewer, it is often not clear how these are weighted and/ or evaluated. The relative merits of particular broader impacts ( <i>i.e.</i> , the training of undergraduates) can seem to vary from panel to panel. Panel discussion helps to balance the weighting of the two merit criteria. The Review Analyses are quite strong and include the summary and recommendation section that clearly outlines the rationale for award or decline. A few proposals, most commonly those before 2017, had shorter PO Comments sections. PO comments have since become more extensive. PO analysis helps to clarify each of the review criteria.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	Yes
In general, the written reviews provide very helpful comments for evaluating and potentially improving the proposals. Some comments (especially those for excellent or poor proposals) are briefer, and in many cases this brevity is justified.	

Some reviews remain focused on describing the proposed research and do not provide a clear evaluation. An emphasis on constructive criticisms across both merit review criteria would assist the PI with revisions.	
There is often not a clear link between the rating given to a proposal (E, V, G, etc.) and the written comments. Providing more guidance to reviewers regarding the use of the ratings might help with this issue.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	Yes
Panel summaries are a palpable strength of the process and serve to compile and evaluate concerns raised in the individual reviews and the panel discussions. Panel summaries usually explain odd ratings (E and F on the same proposal, for example) and also provide the relative ranking of the proposal (High, Medium, or Low Priority). Some summaries are brief but still provide strengths and weaknesses in both criteria. However, others are too brief and not sufficiently informative to understand the rationale for decision.	
Data Source: Jackets	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	Yes
The Review Analysis is an incredibly useful document. This Analysis summarizes all the reviewer comments, considers aspects such as PI funding, and provides a clear justification for the award decision. The program officers are commended for spending significant time to make these documents very clear. In some cases, the Analysis includes suggestions to the PI for improving the proposal. For example, the Jackets contain evidence of an improved CAREER proposal based on PO comments. The PO comments have become noticeably more detailed in recent years, which provides more feedback to the PIs regarding the basis for funding decisions.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	Yes
The PO Comments are good summaries of the Review Analysis and communicate to the PI concerns regarding unfunded proposals. In some cases, especially prior to 2017, these comments are brief. In reviews lacking a Panel Summary, it is important that the PO Comments contain sufficient information regarding the basis for the funding decision. It would be beneficial if the PI could obtain more information about the ranking (top quarter or half?) of the proposal relative to others.	
Data Source: Jackets	

7. Additional comments on the quality and effectiveness of the program's use of merit review process:

The CSDM-B has an appropriate funding rate for the period reviewed (2016-2019), and is slightly above that of NSF CHE. The funding rate has increased in the two most recent years. The main decision factors for the award/decline are: panel ranking, program evaluation, and existing funding or funding incentive/co-funding. This is considered highly appropriate.

The POs are doing a great job in providing careful and thoughtful reviews of the proposals, as well as giving helpful feedback to the PIs.

In general, the PO comments adequately address both review criteria under a "Review Summary" section, and also contain a separate "Recommendation" section that summarizes the rational for the award/decline decision. Decisions for award and decline are very clear from the Review Analysis, and includes the breadth of considerations, including PI funding. Good use of EPSCoR. Continued discussion of what constitutes strong broader impacts is needed.

	SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
	1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	Yes
	The reviewers selected appear to have the appropriate expertise to evaluate the proposals. As an example, proposals in CSDM-B that utilize computational methods are reviewed by panelists with expertise in computational methods <i>and</i> the relevant area of chemistry. There is also good breadth in terms of types of institutions and reviewer gender. The selection of qualified reviewers is a particular challenge for CSDM-B given the breadth of areas considered. In terms of chemistry disciplines under review, CSDM-B is perhaps the most diverse in the Chemistry Division. The program officers are commended for identifying appropriate reviewers for each proposal and composition of review panels.	
	The use of reviewers suggested by the PI seem to be used more in ad hoc reviews. Can more suggested reviewers be incorporated into the panels?	
-	Data Source: Jackets	
	2. Did the program recognize and resolve conflicts of interest when appropriate?	Yes
	The program officers do a good job in resolving COI at the very early stages of the review process.	
	Data Source: Jackets	
	3. Additional comments on reviewer selection:	
	There is a good diversity of reviewers in terms of types of institutions. The panels are more heavily weighted in reviewers from larger, R01 institutions, but the proposals under review also largely come from these types of institutions. The CSDM-B program does a very good job of handling seven panels in different chemistry sub-disciplines.	
	The reviewer database needs to be continually improved, especially to ensure diversity on review panels. POs are encouraged to pursue reviewers from a broad range of areas (industry, international, national labs).	

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

The CSDM-B program has been well managed. A clear outline of funding areas between CSDM-A and CSDM-B have helped PIs in choosing the programs to submit proposals. There were four CSDM-B program officers in 2019, which is appropriate given the increasing number of proposals submitted. The program has also shifted to have a large majority of panel reviews (or panel reviews with additional mail-in reviews) compared to mail-in reviews. This shift would seem to ensure a better review process. The program has obviously been responsive to feedback from the last 2016 COV review. PO comments have also improved over time, as commented on further below. Panel summaries have become more uniform, including strengths and weaknesses categories. Mail-in reviews are now used typically for proposals that do not fit well with a given panel. Given the diversity of the proposals in CSDM-B and the fact that not all proposals could fit into the panels, the program is encouraged to continue using both panel and mail-in reviews. Having a mix of PO's and rotators is a good way to handle the work-loads and maintain continuity within the program.

The program officers' consistent support of CSDM-B fundamental science is very strong. They continue to find opportunities for sustaining transformative fundamental chemical science in the areas of the program. The POs also are efficient in recognizing proposals which lack innovation or significant broader impacts. Analysis of current and pending support is well done, ensuring that no other overlapping funds are already available.

2. Responsiveness of the program to emerging research and education opportunities.

A number of proposals were funded under the SusChem initiatives, which was a special research area. CSDM-B has actively participated in emerging research opportunities such as the NSF's 10 Big Ideas, including Quantum Leap (QL) and Harnessing the Data Revolution (HDR).

CSDM-B has also funded proposals in, e.g., photovoltaics, part of the solar energy research to address the national needs. One young researcher receiving a CAREER grant from the CSDM-B later received a Presidential Early Career Award for Scientists and Engineer (PECASE).

The level of funding for emerging areas should be balanced with funding for ongoing areas. The science must be innovative in all areas (both emerging and ongoing).

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The program officers are doing an excellent job in identifying emerging areas and making good investments in transformative science leading to a diverse portfolio.

This program is largely curiosity-driven and multidisciplinary. The innovation and importance of these research directions are then evaluated by the review panel, leading to selection of competitive proposals for funding. The research portfolio seems to be balanced.

#### 4. Responsiveness of program to previous COV comments and recommendations.

The program has responded well to the previous COV comments. When the 2016 COV review was conducted, the program was moving to mostly panel reviews. The suggestions by the previous COV to improve the panel review process have been adopted by the program. Many reviews are now being accomplished through the panel process, which provide more substantive comments to the PIs. CSDM-B also use ad hoc reviews for those that do not fit a particular panel.

The success rate has improved recently due to limiting the number of proposals per PI. The COV would like to see this funding rate remain constant and if possible, the awards increased in size.

Diversity in awards (geographic, types of institution, gender, URMs) should continue to be a priority. We encourage the POs to continue to seek funding/co-funding from various pools to support proposals that enhance diversity.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

Overall CSDM-B has a well-balanced portfolio, particularly funding projects that are innovative, integrate research and education, are multidisciplinary, and are relevant to NSF's mission and national priorities. The overall funding rate of proposals awarded is higher than the average for other NSF CHE programs. A few projects are co-funded with other programs in CHE (e.g. CMI, CLP, MSN) and other divisions (e.g. MPS-DMR, MPS-OMA and O/D-OIA EPSCoR).

There is a good balance in award size and duration: the average duration is slightly over three years and the average annual dollars are comparable within the Divison. This has been very consistent over the past 4 years. While steady funding should perhaps be expected in the current climate, it must be noted that PI costs are increasing, thus the flat award amounts will at some point be detrimental to research.

There is a good balance in awards to new and early-career investigators: overall the number of awards to new PIs is comparable across the Divsion; for early career investigators the number is slightly higher. The numbers were much lower in 2016 than in other years.

Good balance in geographical distribution of awards: there were more awards to CA, but this might reflect the number of proposals received from this state. CSDM-B receives a relatively low number of proposals compared to other programs and, consequently, its award distribution might more closely follow their submission distribution (this information was not provided).

Good balance in awards to different types of institutions: significant numbers of awards are to Research Intensive PhD Institutions, an a much smaller number are made to PUIs. It is likely that this is a result of the low number of proposals received from PUIs. Also, a relatively large number to non-Research intensive PhD Institutions.

There is a good balance in participation of groups that are underrepresented in science and engineering, and award rates to applicants who are from underrepresented groups are comparable or better than the overall average.

PI's Annual (and Final) Reports in general report multiple products (mainly publications in high ranked journals), training of students at all levels, and other impacts to the community. In particular it was noted that the awards support training of graduate students, post-doctoral scholars, undergraduates, and high school students.

#### **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

Broaden opportunities for collaborative and co-funded proposals, particularly interdisciplinary projects.

Expectations for productivity with prior NSF funding are unclear in the review process.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

How are scientific highlights used by NSF? Can these be used more effectively to educate legislators and the public?

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

Provide and maintain a program-specific reviewer spreadsheet with rankings of the reviewers (*i.e.*, to eliminate repeated selection of reviewers who give poor-quality reviews). Increase award duration to four years for single-investigator proposals. Provide more timely feedback to the PIs. In some cases, PIs only have two to three months to revise proposals.

Continued support of fundamental science is crucial to the mission of NSF.

- 4. Please provide comments on any other issues the COV feels are relevant.
- 5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

COV report could be every five years, rather than four. The COV could be provided with a set of aggregate data regarding the reviewer pool.

#### INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

## CTMC: Chemical Theory, Models and Computational Methods

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

#### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Yes
CTMC is using a combination of ad hoc and panel reviews, providing a fair and succinct evaluation. This makes easier decisions for program managers. Recommendation is to continue and fine-tune the present protocol, particularly given an increased number of virtual panels.	
Sizes of panels should vary in the 6-10 panelist range, 10 being be the upper limit (balance seeing enough vs possibility to evaluate fully each proposal).	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Yes
<ul><li>a) In individual reviews?</li><li>b) In panel summaries?</li><li>c) In Program Officer review analyses?</li></ul>	
Overall, all of the reviews do encompass both criteria. Accumulation of ad hoc reviews is critical as they provide a diversity of reviews. In practice, the panel finesses and summarizes ad hoc reviews as well as their own for consideration by the program manager.	
Notably there is a significant diversity of interpretation of the meaning of the broader impact criterion as far as the ad hoc reviewers. Some reviewers do not address broader impacts adequately. The panel especially is able to balance	

this diversity and put the reviews on a uniform scale. Ultimately, both review criteria are properly addressed in the Program Officer review analyses.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	YES
For the most part. Altogether, the program managers are aware that some reviewers will be laconic and will not provide exhaustive comments on a given proposal-which will obviously not help very much in the review process. It is unclear whether or not the reviewers do not have the time to invest or whether they are do not want to invest in reading a proposal a proposal just far enough outside of their direct expertise. It is good to see reviewers willing to take the time to write extensive, detailed reviews.	
This conundrum is a natural part of the process and while the situation can always be improved, the problem cannot be completely alleviated given the voluntary nature of the review process. All the CTMC can do is to continue to seek the best feedback possible, noting reviewers who do not deliver.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	
Program managers are to be applauded for their honest efforts to combine the diverse and frequently incoherent ad hoc reviews and the feedback from the panel it takes experience and intuition to single out the winners given such heterogeneous input.	
We also approve of the format of the panel summary consisting of explicit brief Strength and Weaknesses sub-sections per each Intellectual merit and Broader impacts criterion: this review seems to work well and provides clear feedback to the PI.	
Data Source: Jackets	YES
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	YES
Overall yes, absolutely! The documentation fairly reflects the essence of the reviews and discussed questions.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	YES / NO
Overall yes. In the case of funded proposal, the feedback should emphasize received criticism and NSF expectations so that the PI's research program is strengthened. At the same time, in the case of a rejection, the feedback should be constructive by pointing the path toward proposal improvement by providing specific (not general!) comments. For the most part, this practice already occurs, but we found that the feedback did depend on who moderated the panel.	
There is very good information in the Review Analysis that the PI never sees. Some of this material should be conveyed to the PI in the PO Comments to help the PI, especially in the case of declines. We realize that there are constraints on what the PO can say about the analysis, but as much information as possible should be conveyed to the PI.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
Our COV panel did discuss in detail the nature of the CAREER selection process. On the one hand, we can see the difficulty of assembling a panel for a diverse set of CAREER proposals. On the other hand, using ad hoc reviewers alone may not necessarily lead to the most fair process. We were not able to come to a clear consensus on the next step forward.	
There are currently not enough standards and guidance on the contents of Data Management Plans. As data storage capacity increases, data management needs and capabilities change. Program Officers should continue to appropriately weigh a wide variety of data management plans while the community continues to develop options. Requirements for making code and data available to the community should be clarified, taking into account the scope and budget of the project.	

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
Largely the program managers are doing an excellent job of selecting appropriate reviewers with a broad expertise encompassing not only the subject matter focus but also a much broader scope of theoretical chemistry.	
The COV applauds CTMC's approach to send early emails to a broad variety of potential referees to get early feedback and secure ad hoc and panel reviewers.	
The COV are also pleased that CTMC has secured expert reviewers not only from academia, but also from national labs and industry (when relevant). Reviewers are geographically diverse. Cultural and gender diversity has improved and should continue to improve.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
The program managers are very keen in identifying and resolving any possible COI at very early stages.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	
Our panel was deeply concerned that a postdoc advisor does not count as a COI.	
The COV recommends moving to four-year award cycles allowing for research programs to engage long-term projects with continuous funding and ensure continuity, allowing for long-term impact as well as reducing the burden on the reviewing community	

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

For many years, the CTMC program has continuously supported and promoted scientific exploration in theoretical and computational chemistry, throughout a series of national initiatives, bubbles and hot subjects that emerge and disappear. We commend the program for its consistency and adherence to the principle of basic scientific discovery aiming to award the best and the brightest researchers and promote long-term transformative chemical science. The program managers are very efficient in identifying proposals that lack innovation, are extremely risky or lacks broader impacts. Moreover, the program managers do a very careful job in analyzing current and pending support of each PI to avoid possible overlaps with other projects. Choice of rotators is indicative of strong effort to achieve balance in expertise and background.

Finally, the COV notes that the CTMC program has actively found significant amounts of co-funding and encourage the program to expand this area particularly taking into account opportunities from the "Endless Frontier Act" (EFA) transforming NSF into "the National Science and Technology Foundation".

2. Responsiveness of the program to emerging research and education opportunities.

The program does respond to emergent opportunities. For instance, we have seen an immediate increase of investments into the quantum and data science areas following national calls. Having said this, it is essential that one not replace or compromise the existing commitment to excellence in science with a rush to hot areas -- such a compromise would necessarily inflict irreparable damage to the traditional core of this program. The program managers seemingly are flexible enough to follow and promote these emerging areas of science, and they are able to ensure proper quality control for funded proposals. The program works well with other divisions to support interdisciplinary work and emerging areas.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

This program supports the development of basic new scientific concepts and enabling theories and technologies and thus will inevitably spawn other research in priority areas. In fact, we commend the agility and willingness of program managers to identify and prioritize transformative science areas leading to the diverse portfolio. The benefits of the supported work may be realized in the long term; we feel that this is quite appropriate for this program.
## 4. Responsiveness of program to previous COV comments and recommendations.

First and foremost, the success rate has increased to a near optimal range – in this range, one can both fund and require good science. We believe this increase is due to a combination of several factors, including better funding and limitations on the number of proposal submissions from a single PI in a given year. This increase in success rate was one of the major recommendations of the previous COV and was addressed properly.

With regards to funding per award, there has been an appropriate slight increase in the average award size so as to take into account inflation, which does result in a steady or slightly increased buying power per proposal, again addressing the previous COV recommendation of maintaining/increasing the monetary award value. Overall, a recommendation for future investment is to keep the present success rate constant, and if possible, increase the monetary value per award (budget allowed).

The panel review system is functioning smoothly at this point and has improved. CTMC seems to be better at identifying methods proposals – and routing them correctly – than in the previous COV review period. Applications proposals are reviewed elsewhere so that this program can rightly focus on method development projects.

Finally, the previous CTMC COV made recommendations regarding how to evaluate the past experience of the submitting PI; the COV asked that the PI be evaluated both on the basis of overall past performance as well as on the basis of their performance over the last NSF cycle. This request generated a great deal of discussion within the present committee, and it is not clear to some of us that this recommendation was taken to heart. Our committee does understand that this question of evaluating past PI performance is complicated.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

## **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

For PUIs, the COV suggests giving smaller awards, but more awards as a way to engage a wider group of students and faculty.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

The COV recommends moving to four-year award cycles allowing for research programs to engage long-term projects with continuous funding and ensure continuity, allowing for long-term impact as well as reducing the burden on the reviewing community.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

The COV believes there should be more proactive efforts to engage persons from underrepresented groups, through collaboration between the research and education directorates.

In addition, if additional resources become available, such as coming from the EFA initiative, the COV would recommend the establishment of long-term programs under CHEM Division focused on developing capabilities such as open-source software, synthetic protocols, databases, specific technologies, etc. Examples of such capabilities would be DOE long-term supported software packages such LAMMPS and NWChem.

4. Please provide comments on any other issues the COV feels are relevant.

The overall question of how to encourage and promote a diverse group of chemists in the USA is almost certainly beyond the scope of the CTMC program but the Chemistry Division as a whole should be more proactive in broadening participation.

CTMC supports important fundamental science, the impact – often highly significant - of which is realized down the road, as opposed to more immediate applications.

5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

The COV panelists all found multiple password logins as onerous.

## INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

## **ECS: Environmental and Chemical Sciences**

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

## I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	YES
Panels have been the most effective review method, which is especially reflected in the panel summaries. The discussion of panels, reflected in the summaries, added a tremendous benefit to the review process by enhancing or downgrading merit review criteria evaluations of individual reviewers to provide a fair process. The previous comment is especially valid in cases where a few individual reviews from ad-hoc reviewers lacked calibration relative to the overall panel outcome. Overall, the COV notes that panels are more effective for securing balanced review summaries, as panelists can argue more effectively to fund or not fund certain proposals based on both merit review criteria. This interdisciplinary program does an excellent job of providing panel summaries to the PIs (306/333 for 2016-2019), which is important for transparency in the review process.	
2. Are both merit review criteria addressed	YES
a) In individual reviews?	
b) In panel summaries?	
c) In Program Officer review analyses?	
1. In general, individual reviews have provided detailed evaluation of both review criteria but a few reviews of lesser quality were noted. In a few	

cases, PIs suggested relatively weak solutions for promoting broad participation and individual reviewers should have more carefully examined the thoughtfulness of these ideas. In addition, we noted that individual reviewers may be insensitive to the fundamental nature of the research performed in the ECS program; panels and ad hoc reviewers should be reminded of this before tackling their review work.	
<ol><li>Panel summaries clearly addressed both review criteria and better reflected on the broader impacts.</li></ol>	
3. Program Officer (PO) review analyses incorporated both review criteria and reflected on the panel outcome and summaries. There were a few cases of GOALI and CAREER proposals that would have benefitted further by the analysis of a panel. Overall, panels are recognized as the best way to facilitate a fair evaluation and provide elements for a standardization for the decision analysis by the PO.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	YES
In general, the quality of scientific feedback provided by reviewers has improved from previous COV reports, and this is the case, especially, for the intellectual merit review criteria. Indeed, the evaluation of CAREER proposals exemplifies the best assessment that PIs could receive of their proposals. The excellent feedback provided by reviewers of CAREER proposals is a major contribution to the scientific and educational outcomes of this program.	
The reviewers were from different departments and not only chemistry. For example, there were different types of engineering departments reviewing chemistry proposals and they should be reminded to provided consistent evaluations with a fundamental molecular level focus. There was some disparity in the reviews that reflected the philosophy of their respective formal education and current department/field (e.g., engineering or geology, environmental science).	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	YES
Panel summaries were clearly written and, when needed, prioritized explaining any fatal flaws for jackets that were placed in medium priority or low priority rankings.	
Because the makeup of the panels including different subdisciplines, the rational recommendation for funding was justified. Several times a consensus was not noticed before the panel met, just from individual reviews. Constructive	

critique was used to reach a final conclusion of the rankings of the proposals during panels. It would be good to remind reviewers they can modify their ratings and individual reviews as part of the panel final decision, while keeping their own opinions. The panel summaries were informative regarding their decisions and provided the PI with the most useful comments for revision and resubmission. <b>Data Source: Jackets</b>	
5. Does the documentation in the jacket provide the rationale for the award/decline decision? The documentation in the jacket provided an impressive summary of both the work proposed and the discussion of the panel/reviews. The review analyses demonstrate excellent assembly of panel and ad-hoc reviews; as well as, in a few cases, searching for alternative programs in and out of the division when proposals did not fit within the program description or were not recommended for funding. The review analyses also reflect that the PIs have typically asked for strictly needed funding, and that the Program Officer is keeping excellent control of its budget by monitoring the rate of spending of awards soliciting supplements.	YES
The COV appreciated the PO's effort to contextualize in the review summary the process and provide rationale for the decision. The review analysis was often the most informative document in the jacket, as many proposals were reviewed very differently (e.g., using the whole spectrum of ratings) as a result of the variety of reviewer scientific disciplines and opinions.	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	YES
The documentation provided to the PI does an excellent job providing the rationale for awards and decline decisions. However, the COV felt that the review analyses, which are not provided to the PI, were the most informative documents with regard to the decision. Although parts of this information are given in multiple areas (reviews, panel summaries, PO comments), it would be helpful for the PI, if possible, to see this document.	
Providing a post panel ranking as an addendum to the overall review process would also be helpful.	
Data Source. Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	

This program is impressive in that it is able to navigate multiple disciplines and approaches to chemistry. The program focus on fundamental chemistry and hypothesis driven proposals distinguishes it from those in other divisions. This effort is made clear in the breadth of the ECS portfolio.	
It is important to highlight that the Program Officer's work enabled an appropriate balance of the portfolio of the ECS program. The COV appreciates the effort made by the Program Officer to re-evaluate anything that individual reviewers could have mistakenly included in their comments before they are released, even identifying a mistake in one review that was corrected in the Review Analysis.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
Yes, the program assembled panels that included individuals with the appropriate expertise to evaluate the intellectual merit of each proposal well. In addition to researchers in chemistry departments, many colleagues from engineering departments as well as geology, and environmental sciences participated in the review of jackets. This extended pool of reviewers contributes to the challenging task of evaluating many proposals that include both experimental and computational modeling. Panel reviews were supplemented with ad-hoc reviews to ensure that all proposals were evaluated thoroughly. The Program Officers worked to incorporate PI recommended reviewers, especially for ad hoc reviews. The demonstrated effort of the program to review all proposals with the appropriate expertise was extraordinary.	
The COV members encourage the PO to continue to recruit chemists for the review process, as this is a CHE program. Similarly, the COV encourages the PO to remind the reviewers and panelists of the molecular level goal for evaluating for this program. Reviewers from other fields provided the technical expertise needed to fully assess the proposals.	
The program was not as successful in identifying panelists well-qualified to evaluate the broader impact criteria. This is to be expected in that this criterion is still relatively new and investigators are working to define what constitutes a well-developed plan for broader impact.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
The e-jackets contain evidence of panelists recusing themselves from discussion of select proposals and declining requests to review. Both provide evidence that ECS has handled conflict-of-interest appropriately. Data Source: Jackets	
3. Additional comments on reviewer selection:	

# **III.** Questions concerning the management of the program under review. Please comment on the following:

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

## 1. Management of the program.

The management of the program is clearly engaged in both the oversight of the portfolio and the individual proposal review process. In the examples provided in eJacket, it was clear that management thoughtfully considered panel and ad hoc reviewer comments as well as the appropriateness of the proposal in the ECS portfolio when making funding decisions. In the case of one "Return Without Review," management did due diligence to ensure the proposal did not fit under other NSF programs before making the final decision to return it.

The COV commends the PO for navigating this multidisciplinary program. The PO's call for chemistry and hypothesis-driven proposals, not field work proposals, is an excellent way to focus this program to provide funding to impactful science. The COV also commends the PO for being an excellent steward of NSF funds: if a proposal doesn't fall squarely in the ECS domain, they ask for collaboration between programs or find other sources of funding. The PO is also vigilant about funding timing, which is important in stretching the funds of a small program such as this. When a PI has money from a previous grant she timed the new grants to start after figuring out when the money from the previous grant would run out.

PO is transparent about leveraging connections within NSF and acquiring funding from other sources to fund as many ECS proposals as possible. Which proposals are funded is dictated in part by the ancillary funding sources.

2. Responsiveness of the program to emerging research and education opportunities.

High quality proposals were funded. There were a wide range of proposal types that were supported.

As in 2016, emerging research was largely defined by the ECS community and by the proposals that were submitted.

No RAPID applications were either requested or included in the proposals provided in eJacket, so it is difficult to comment on the responsiveness of the program to rapid turnaround requests.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

Overall, the program is responsive to internal prioritization processes as demonstrated by strong alignment with the ECS Program Description as well as funding of proposals in Data-Driven Discovery Science in Chemistry (D3SC) and Innovations at the Nexus of Food, Energy and Water (INFEWS). This is a small program; the COV would like to see more funding provided to it, as there were some well-evaluated proposals that couldn't be funded due to portfolio distribution and budget limitations.

4. Responsiveness of program to previous COV comments and recommendations.

While the program has generally been responsive, there was a notable comment from the 2016 COV regarding the size of the average grant compared to the average for the Chemistry Division. The average amount of an ECS award remains smaller than the average for the Division, although the Median Annualized Amount for ECS is larger than for the Division. The general sense is that PIs are asking for what they feel they need to execute, so this is not a particular concern for the 2020 COV.

One of the major concerns of the 2016 COV was the uneven reviewer base (chemistry vs. other disciplines) and the quality of reviews. This really seems to have been addressed, as most of the reviews seen by the COV were very informative.

Another concern was that the community seems to be confused about broader impacts and how to evaluate them. This seems to still be an issue, as different disciplines will regard these differently and place different weight on certain things, but the PO has done a good job to synthesize the various thoughts of reviewers into a cohesive message.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

Highlights from CHE awards, project reports and outcomes, demonstrate the ECS program is providing scientific contributions with molecular level understanding and computational work, to a very interdisciplinary field. This interdisciplinary field has close connections to programs in the Directorates of Engineering and Geosciences, which benefit from the key molecular level understanding generated by this program. These chemistry contributions to the Division are evaluated as outstanding for the relative low level of funding per award.

The ECS program is interdisciplinary in nature. Consequently, the program has worked to focus the types of proposal funded by ECS by modifying the program description to specify systems are to be understood at a molecular level. Field measurements and pure instrumental design proposals are discouraged from applying to the ECS program. In many cases, proposals are redirected to different divisions by the program officer.

This being said, the program does work to co-fund proposals that have both a molecular perspective and a complement more appropriate for another directorate. Many proposals within the atmospheric science community are co-funded by engineering and geosciences.

The Division supports engagement of the community through the inclusive selection of reviewers. It does a good job of sharing funding opportunities with investigators via CHE Newsletters and other electronic correspondence.

Targeted correspondence to better engage investigators that are underrepresented in the ECS community is merited. Including new investigators on reviews as is done already can be complemented by better advertisement of workshops that are available to help new investigators compile their first NSF proposals and/or revise declined proposals. Partnering with professional societies such as the NSF-sponsored receptions at national American Chemical Society meetings is an effective way to do this and should be continued.

## **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

The members of the COV favor the utilization of panels over ad-hoc reviewers when seeking for recommendations for awards and decline decisions. Panels are a key instrument to advance the discussion of proposals and perhaps some version of minireview panels could be implemented to avoid making decisions purely based on mail in reviews for calls that do not merit gathering a full panel.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

The COV commends the work performed and recommend sharing the keys for success with other programs and agencies to benefit the larger community.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

The average grant budget awarded should be evaluated to determine whether it should be made larger to match other Division of Chemistry programs.

4. Please provide comments on any other issues the COV feels are relevant.

There were some concerns about meeting the full representation of the portfolio by states, by calls for proposals, etc. Perhaps, by increasing the outreach of NSF in unfunded states (e.g., with new investigator workshops) there would be an advancement in this field.

5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

This is the first all-virtual COV review, and it is impressive how well NSF has brought it together. A large virtual meeting can be extremely challenging but this one has been well run and well organized.

## INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

#### **MRI: Major Research Instrumentation**

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

#### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
<ol> <li>Are the review methods (for example, panel, ad hoc, site visits) appropriate?</li> <li>Panel/telepanel reviews are suggested whenever possible.</li> <li>Ad hoc reviewers should only be used if necessary (due to expertise or travel restriction).</li> </ol>	Yes for PhD Granting Institutions and sometimes for PUI
Panel review strengths: lengthy discussion of merits and relative rankings, reviews submitted on time.	
Ad hoc strengths: Expertise is utilized, good option if travel or telepanel is not possible.	
Ad hoc disadvantages: Late/not returned submissions.	
Note: there was a sharp decrease in ad hoc reviewers requested for FY18. Is there a specific reason for this? Or, is this an intended trend by the Program to use more panels/less ad hoc?	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Yes
a) In individual reviews?	Yes
b) In panel summaries?	Yes

c) In Program Officer review analyses?	
<ul> <li>Individual reviewers addressed both criteria well (generally), with IMs being better addressed.</li> </ul>	
<ul> <li>Panel summaries adequately addressed both criteria.</li> </ul>	
<ul> <li>PO review analyses were very descriptive for both criteria.</li> </ul>	
For the most part, BIs were discussed thoroughly in reviews. However, some reviewers did not give it as much attention as IMs. Given the unique nature of the MRI program (expectations for shared users and education), more emphasis and weight should be given to the broader impact rating/ranking/comments from the reviewers and from the program manager when award/decline decisions are made. The COV recommends a revision of the review template to better solicit balanced BI and IM information.	
The balance in review of the two merit review criteria did not vary significantly between funded and declined proposals. The panel summaries are consistent between these two groups.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	Yes
In general, reviewers were excellent with their comments giving the PI suggestions, questions, and criticisms when deemed appropriate. In a few cases a lack of substantive information was noticed in the review.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	Yes
In general, panel summaries were written accurately and reflected individual reviews and panel discussion.	
In multiple cases, the individual reviews showed overall enthusiasm for funding, but views were changed in panel discussions. Unfortunately, final documentation given to the PI included reviews with high ratings and a panel summary that details reasons for not recommending funding. It might be prudent to provide a post-panel discussion score if a major decision has been altered to help make message to PI more consistent.	
Data Source: Jackets	

5. Does the documentation in the jacket provide the rationale for the award/decline decision?	Yes
In our opinion, this is a resounding YES. There is an abundance of information in the jacket (for NSF staff) to document the decision made. The review analyses, in particular, were written with plenty of detail and justification. The review analysis, by far, was the document that provided the most comprehensive and transparent look at why a proposal was funded/declined.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	Yes
It was appreciated that the COV could see the panel ranking of proposals in the Review Analysis as part of the explanation of the decision recommendation and encourage the PO to provide even more detail from the review analysis in the PO Comments section. The PO Comments section should also be emphasized to make it more visible to PI.	
The documentation to the PI provided information relative to the review process. The extent to which the PO went to secure additional funds (which is directly related to the ability to make an award) might be underemphasized. If PIs were to more fully understand the lengths the PO goes to outside of the MRI budget, it might make the community appreciate the opportunities provided more. <b>Data Source: Jackets</b>	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
The panel memo provided by the MRI program for each year was very helpful in framing the overall program.	
The Review Analysis provided for the MRI program was detailed and thorough, which consistently provided a clear picture of the history of review for each proposal.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	Yes
In our opinion, the reviewers selected were generally appropriate with expertise in the field and currently active in their discipline. Proposals were grouped by instrument type, so panels typically had strong expertise in a given area, both in terms of assigned reviewers and additional panel members. The Program also utilized a good balance of reviewers from PUI and PhD institutions. However, the members thought it would be helpful to include more women and URMs as reviewers.	
We noted that reviewers requested by PIs were often not utilized.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	Yes
MRI does a good job at monitoring and avoiding conflicts as the numbers presented are very low.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	
A reviewer database is utilized for the selection of reviewers. The database information had been expanded, as was suggested in the 2016 COV report. This database should continue to be developed. It would be useful to the community to know the mechanism for how people are included in the database and how reviewers are chosen.	
While we appreciate the effort of the PO to assemble a diverse group of reviewers, there were panels that lacked diversity. The COV members encourage strategies to ensure the involvement of more women and URMs. There is balanced representation between PUI and PhD granting institutions, relative to the distribution of proposals. However, there is some perception of an imbalance in reviewer expectations for PUIs.	
The reviewers appeared to be very aware of budgets relative to the experimental need.	

# **III. Questions concerning the management of the program under review**. Please comment on the following:

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

POs are encouraged to keep utilizing an expanded reviewer database to select the best referees with specific expertise while retaining diversity.

The PO consistency in the MRI Program is commendable. Having a permanent and a rotating technical scientist is important to the continuity of Program. It is also important to have a scientist in training to cover any gaps.

The MRI Program is well managed. Panels are used whenever possible, COIs are low, funding levels are comparable to the rest of the Division (regardless of number of proposals or funds received), average annual dollars remains consistent, and funding of new PIs remains consistent as well.

A strength of the program is the time the PO commits to corresponding with PIs to address any issues or questions. The PO is also commended for seeking additional funds from other NSF programs to enable the funding of more instruments.

There is an occasional example where funding was not recommended for a given proposal; however, few specifics about why that recommendation was made were provided to the PI. Although these are outliers in the eJacket program portfolio, the COV notes that it is critical that the PO provide justification for not funding the proposal regardless of the reasoning.

While PUI and PhD granting institutions are considered separately, the funding rates for the PUI are significantly lower than the PhD granting. The MRI program faces different budgetary guidance for distribution of funds between PUI/PhD institutions and the POs try to manage this effectively.

2. Responsiveness of the program to emerging research and education opportunities.

There are few instrument development proposals (Track II). It would be nice to see the Program encourage more submissions of developmental proposals. If instrument development proposals were more prevalent, special initiatives - e.g. the BRAIN initiative, CDS&E, etc. - might be suitable routes in emerging areas. A mechanism to encourage instrument development proposals as opposed to acquisitions proposals – would encourage the most emergent instrumentation research.

ChemMatCARS is exceptional in bringing in experimental and emerging science via their mission.

Acquisitions to enhance existing research infrastructure or to replace aging equipment were judged to facilitate emerging research and education, where more current and up-to-date equipment is necessary.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The program is funding a range of instrument acquisitions within the scope of their submissions. The portfolio seems to be balanced across areas such as gender, race, ethnicity, geography, type of institution, type of research, and new and early-career investigators. We note that some COV members felt that there were too few proposals with new investigator co-PIs - this is something that should be encouraged to help new colleagues launch their research programs. The RAs suggest a trend that the PM provides very clear direction to the panels and useful feedback to the PIs.

Looking at the data, the success rates for 4-year and MS institutions are much lower than PhDgranting (often the percent funded is less than half of the PhD-granting institutions for MS institutions, and several-fold lower when considering only 4-year schools).

- The MRI program in Chemistry is usually more successful at getting co-funding for proposals from the PhD-granting institutions. Perhaps the funds that come specifically from the MRI program should be even more heavily weighted to PUIs than they have been in the past.
- Approximately the same number of proposals come from each group type each year, which means that significantly fewer PUIs are getting instrumentation they probably really need.

It is important to note that a very large portion of underrepresented students are educated at PUIs. If the NSF wants to truly advance the cause of broadening representation of underrepresented groups in STEM, those schools need to have the instrumentation to allow students to participate in research or get hands-on experience with instruments in courses, which will then enhance their enthusiasm for continuing their STEM education.

## 4. Responsiveness of program to previous COV comments and recommendations.

The 2016 COV recommended CHE to advocate for more funding overall and to maintain focus on high impact fundamental research. As the overall budget for MRI is a function of the NSF budget, CHE should continue to strive for increased funding for the MRI program. The previous COV urged the Division to enhance transparency of the review and decision process. The MRI program does an exceptional job overall corresponding with PIs and most panel summaries are reflective of panel discussions and decisions.

They urged the Division to broaden the representation of proposals across types of institutions and PIs. For the MRI program it should be noted that FY2019 saw an overall decrease of submitted proposals from all types of institutions. With that said, the total number of proposals received from PhD institutions has remained fairly constant while PUI submissions have seen a dramatic decrease throughout the 4-year span. It is important to keep looking for creative ways to interact and encourage the PUI community.

Involvement of women and URMs have stayed fairly constant throughout the 4-year period (33% and 31%, respectively). However, the funding rate for these proposals is about 5% lower than those that have no underrepresented groups. This is somewhat problematic. The COV members would like to see an increase in the number of awards to women, URMs and HBCUs. Approaches to improve participation from these groups should be prioritized.

In one RA, the PO has stated that he would follow up on proposed deliverables related to broader impacts. This practice is highly encouraged and should be more widely adopted.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

RESULTING PORTFOLIO OF AWARDS	APPROPRIATE, NOT APPROPRIATE, OR DATA NOT AVAILABLE
1. Does the program portfolio have an appropriate balance of awards across disciplines and sub-disciplines of the activity?	Yes
Different areas of analytical chemistry were funded with majority being NMR and Mass spec. Only a few instruments such as Raman and custom-made instruments were in the portfolio of jackets that the COV had access to.	
Data Source: EIS/Committee of Visitors Module. From the Report View drop-down, select the Funding Rate module to see counts of proposals and awards for programs. The Proposal Count by Type Report View will also provide a summary of proposals by program.	
2. Are awards appropriate in size and duration for the scope of the projects?	Yes
The instruments are expensive and the awards reflect this.	
Data Source: EIS/Committee of Visitors Module. From the Report View drop-down, select Average Award Size and Duration.	
3. Does the program portfolio include awards for projects that are innovative or potentially transformative?	Yes
There were a few proposals instrument development proposals and some proposals had novel uses of the requested instrumentation.	
Data Source: Jackets	
4. Does the program portfolio include inter- and multi-disciplinary projects?	Yes
There were several cases where the instrumentation was used across different disciplines even though not exclusively chemistry.	
Data Source: If co-funding is a desired proxy for measuring inter- and multi-disciplinary projects, the Co-Funding from Contributing Orgs and Co-Funding Contributed to Recipient Orgs reports can be obtained using the EIS/Committee of Visitors Module. They are available as selections on the Report View drop-down.	

5. Does the program portfolio have an appropriate geographical distribution of Principal Investigators?	No
This was the only disappointment in the COV that was a shocker. California, New York, and Pennsylvania were the major awardees. This may be due to the size of these states and the number of world class research institutes. NSF should try to get more participants from the Midwest and Southern states. Statistics should be reported relative to the number of proposals submitted. Geographical representations for both proposals submitted and awards received would provide a better overview of the data	
Data Source: EIS/Committee of Visitors Module. Select Proposals by State from the Report View drop-down.	
6. Does the program portfolio have an appropriate balance of awards to different types of institutions?	No
Mainly large institutions are funded more than smaller ones.	
Data Source: EIS/Committee of Visitors Module. Select Proposals by Institution Type from the Report View drop-down. Also, the Obligations by Institution Type will provide information on the funding to institutions by type.	
7. Does the program portfolio have an appropriate balance of awards to new and early-career investigators? This is due to experience and the success rate was shown to be 25%. However, NSF should have statistics on re-submissions of these rejected proposals.	No
NOTE: A new investigator is an individual who has not served as the PI or Co- PI on any award from NSF (with the exception of doctoral dissertation awards, graduate or post-doctoral fellowships, research planning grants, or conferences, symposia and workshop grants.) An early-career investigator is defined as someone within seven years of receiving his or her last degree at the time of the award.	
Data Source: EIS/Committee of Visitors Module. Select Funding Rate from the Report View drop-down. After this report is run, use the Category Filter button to select New PI for the PI Status filter or New Involvement (PIs & coPIs) = Yes.	
8. Does the program portfolio include projects that integrate research and education?	Yes
Instruments were used in both research and education.	
Data Source: Jackets	

9. Does the program portfolio have appropriate participation of underrepresented groups <sup>1</sup> ?	Yes
The success rate is on par with the regular portfolio.	
Data Source: EIS/Committee of Visitors Module. Select Funding Rate from the Report View drop-down. After this report is run, use the Category Filter button to select Women Involvement = Yes or Minority Involvement = Yes to apply the appropriate filters.	
10. Is the program relevant to national priorities, agency mission, relevant fields and other constituent needs? Include citations of relevant external reports.	No
Data Source: Jackets	
11. Additional comments on the quality of the projects or the balance of the portfolio:	
There were several interesting proposals that were funded.	

# **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

The COV members want to emphasize how important it is to provide transparent feedback to PIs. It is a crucial part of their ultimate success in proposal funding.

Geographical representations for both proposals submitted and awards received would provide a better overview of the data.

The funding seems to be by hit or miss depending on the panel. For example, proposals in one panel had a higher score and was not funded whereas a proposal in a small panel with lower score was funded. It should be possible that the PO could change this and perhaps hold out some funds to account for this discrepancy.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

The MRI program is, in our opinion, meeting the goals of increasing access to instrumentation to advance fundamental science and emerging technologies.

3. Please identify agency-wide issues that should be addressed by NSF to help

As described above, reviewer and PI diversity should be prioritized.

There was a recognized concern about encouraging submissions from HBCUs, HSIs, and Tribal Colleges for instrument funding. It would be great if NSF had some kind of grant writing skills course.

5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

COV templates should be streamlined so members are focusing on the correct version.

A descriptive flowchart of the COV process would be helpful.

A summary analysis/list of the expected and proposed outcomes (number of participating students, presentations by students and PIs, publications, noteworthy research highlights, etc.) resulting from the awarded proposals would have been useful to the COV to assess impact and productivity of the awards. While this data is available to NSF from the annual reports and the COV members can, indeed, search within the annual reports within the jackets to find the information, this is somewhat time-consuming and cumbersome. If there was a more accessible repository of the outcome data in summary form (similar to the stats provided for funding rates by area), this would facilitate the COV in future years.

Providing one hour to write the report for the second program review is too short. We recommend at least 1.5 hours.

## INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

## MSN: Macromolecular, Supramolecular, and Nanochemistry

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

## I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	Yes
Review methods included panels and ad-hoc reviews. About 78% of proposals to the MSN program were reviewed at a panel, a comparatively low number vs NSF CHE as a whole. The COV acknowledges that this is the largest program within chemistry, however, a higher percentage of proposals should be reviewed by panel whenever possible. Panels are suggested whenever possible, as they allow for more in depth discussion of a proposal's strengths and weaknesses. Further, panel discussions more often lead to consensus and relative rankings.	
A few ad hoc reviewers tend to turn in their comments late, or not at all. A relatively large number of reviewers decline to submit a review. In addition to doing their job on time, panel reviewers additionally benefit from in panel training prior to discussion(s). During panel discussion, reviewers get to hear other viewpoints they may or may not have considered. Ad hoc reviews are often used to reach out to particular expertise about certain areas, when needed, to augment the review process.	
Overall, MSN used a combined method of onsite and virtual panels and ad hoc mail reviews, which is appropriate. The program handles a large number of submissions and the COV appreciates the review system as healthy. We recommend that proposals be reviewed as often as possible within a panel; currently, the need for virtual panels is apparent as we recognize them as valuable regarding the scientific content. However, the COV recommends that the onsite panels be maintained if possible because of the networking value of these panels specially for early career faculty.	

Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	Yes
Yes, although a cautionary tale is that reviews/reviewers tend to focus more, or place more emphasis on, intellectual merit. Broader impact reviews tend to be more superficial.	
a) In individual reviews?	
Yes.	
b) In panel summaries?	
Yes.	
c) In Program Officer review analyses?	
This program did a particularly good job at providing a clear rationale for proposal ranking in each case. This is a strength of the MSN program, as it helps principal investigators (PIs) better understand how their proposals and ideas were perceived.	
The broader impacts part is very variable and there is less guidance regarding this part. We appreciate that the program officers respond more to detailed reviews. However, we recommend that reviewers be given guidance to note the rationale behind strong reviews, even if they are strongly positive.	
The review analysis is the most detailed, in-depth document describing why a proposal was or not funded, and/or how close it got to being funded. Perhaps the program could think of providing more information from this document to the PIs, in the form of PO comments, so PIs could get better information about the strengths and weaknesses of their proposal, as received/discussed by reviewers. This will help junior faculty to further develop their proposal and increase success rate.	
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	Yes
Yes, they do, however much more attention is given to intellectual merit aspects. Many reviews do not address or only briefly address broader impacts.	
Yes, these are helpful in further improving the intellectual merit portion(s) of the proposal. However, broader impacts are perceived differently at different	

institutions. Some proposals rated as excellent (E) only briefly discuss or address broader impacts.	
A minimum of three reviews were provided for each proposal.	
Overall, the COV recommends that reviewers be reminded about the value of detailed constructive reviews to help improve proposals specially for less experience faculty. The COV found that panelists' reviews tended to be shorter than ad hoc reviews.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	Yes
Generally, yes. Some COV members recommend that in cases where the initial individual reviews do not match the essence of the panel summary, this should be stated to the PI. This feedback may be even more important when proposals are not reviewed by a panel. It might be prudent to provide a post-panel discussion score if a major decision has been altered to help convey the message to PI and make the process more transparent.	
Some COV members pointed out that data showed that reviewers looked more critically at proposals in a panel. This stresses the need for panel reviews for most proposals, whenever possible. For example, proposals can be declined for programmatic reasons; in some cases, even when having multiple excellent (E) ratings. A panel is better able to discuss this situation, and to provide a rationale for the final ranking and recommendation.	
The COV noted that individual (initial and/or ad-hoc) reviews sometimes fail to divide their feedback into strengths and weaknesses.	
The COV agrees that program officers are to be commended on the quality of the panel summary.	
Data Source: Jackets	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	Yes
Yes, resoundingly. Program officer (PO) comments, context statements, review analysis, and other documentation gave clear indication for the rationale behind each award decision.	
Additional information in the e-jackets often explained why decisions did not always agree with proposal reviews. For example, when proposals were sent to other programs based on the program's portfolio, or when a single PI was already funded by the same program.	

The program often seeks and succeeds at finding opportunities to co-fund highly rated proposals across programs and across directorates, for example with ENG, PHY, or DMR.
Overall, the review analysis was found to be comprehensive. The COV found that the program officers document their rationale for the decisions they reach.
Data Source: Jackets

6. Does the documentation to the PI provide the rationale for the award/decline decision?	Yes
Yes, see above/as noted above.	
We recognize the need to prioritize funding and balance the program's research portfolio. The COV noted some proposals declined for reasons of prior funding from NSF or other agencies. The COV recommends that policy about funding history be made clear to the research community. Once more, providing more information from the review analysis, even if in a consolidated form as PO comments, would be helpful.	
Whenever possible, proposals should be reviewed in a panel, as this provides more critical feedback to the PIs on relative ranking and how to approach resubmissions and future applications. This is particularly important for junior faculty.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
The program should continue to seek opportunities to co-fund proposals when they are reviewed favorably (high or medium priority), along with partnering other programs/divisions, the EPSCOR program, etc.	
The NSF could help the community by defining priorities and posting guidelines for broader impacts in proposals. The COV suggests that these guidelines will make the review process more consistent and will help new investigators.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	Yes
The program utilized a good balance of reviewers from both research intensive/PhD-level, as well as primarily undergraduate institutions (PUIs). It should continue to emphasize panel over ad-hoc only reviews to allow for discussion of proposal strengths and weaknesses and relative proposal rankings.	
Reviewers were selected from a combination of experts suggested by PIs, other PIs previously funded by program, experts in the area, and new reviewers. Having junior faculty serving on the panel helps them to further develop their science and help with the success of future proposals.	
Overall, the COV found that the reviewers were experts in their field, and that the program officers make a commendable effort to ensure a diverse composition of reviews. For example, when the topic of the proposal required it, reviews came from experts across different fields, and when evaluating a proposal from a PUI the reviewers included faculty from similar institutions.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	Yes
Yes, these were identified and handled appropriately. Again, more panel reviews and associated review training would ensure that reviewers are well trained on conflict of interest (COI) minimization.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	Yes
The reviewers are carefully chosen based on their broad expertise. Perhaps indicative of other programs across the division, the program could benefit from having a more gender-balanced set of reviewers. We recognize this is difficult based on the number (fraction) of women scientists in the discipline.	

The COV recognizes the challenges in obtaining a comparable number of	
reviews for the different proposals. The COV noted that a reviewer database	
could be helpful in selecting and to prevent reviewers that are conflicted. A well-	
maintained database will prevent individuals with a past of scientific misconduct	
from being contacted to review proposals.	

# **III.** Questions concerning the management of the program under review. Please comment on the following:

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

The program is to be commended for maintaining a consistent PO lead, along with a team of multiple rotating scientists, all of whom are a strength. The team of 5-6 POs in the program provides stability and consistency over time.

The program manages a large number of proposals (most submissions and most awards) across a diverse scientific portfolio. The topics of the program have adapted and the COV recognizes how well the program officers balance the research areas and how they evolve within their disciplines.

2. Responsiveness of the program to emerging research and education opportunities.

The program description is very clear, outlining the types of proposals that are funded by MSN. It emphasizes experiment and theory, and synergies between them, and proposals that address national needs within the NSF's Ten Big Ideas. The MSN program has a track record of responding to emerging research opportunities within the program's research areas. However, the COV believes that it will be beneficial to have more guidance regarding educational opportunities, for example, suggesting some of the educational opportunities to seed new broader impact activities for the MSN scientific community.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

The COV feels that they did not have enough documentation to judge the development of the research goals of the portfolio. The program has been able to maintain a healthy funding rate, close to the average for the Division. The funding rate was higher in 2019, perhaps as a result of the lower number of proposals managed by MSN in 2019.

The portfolio seems to be balanced in terms of gender. New PI funding rates and those for URMs are lower compared to the rest of the division. Efforts in the past year have improved these numbers. These efforts, as well as those to better train new PIs and URM PIs in the expectations of the program, should be continued and enhanced.

4. Responsiveness of program to previous COV comments and recommendations.

Most previous recommendation have been met.

The COV reviewed the response to the 2016 COV and found that the points were addressed. however, although the NSF Chemistry Division has substantially addressed the points raised by the prior COV, the materials generated are not well advertised. Perhaps direct links to these resources could be in the MSN webpage. The NSF program would benefit from encouraging PI's engagement with the NSF when writing proposals.

As a reminder, more information from the review analyses should be provided to the PIs, at least in the form of more detailed PO comments. Increased use of panels will provide PIs with useful panel summaries.

In light that MSN is the largest program in the chemistry division, the program is clearly generating interest among the scientific community. Therefore, the COV believes that the size or duration of grants should increase. The COV believes that a formal renewal mechanism should be considered as part of the funding options.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

Overall MSN has a well-balanced portfolio, particularly funding projects that are innovative, integrate research and education, and that are relevant to NSF's mission and national priorities. A good number of projects are inter- and multi-disciplinary co-funded with other programs in CHE (e.g. CSDM-A, CMI, CAT) and other divisions (e.g. MPS-DMR, MPS-OMA and O/D EPSCoR).

There is a good balance in award size and duration: the average duration exceeds 3 years and the average annual award size is comparable across the Division. This has been very consistent over the past 4 years. There is a good balance in awards to new and early-career investigator, and this number has been consistent over the past 4 years. For early career investigators the number is slightly higher. There is also a good balance in geographical distribution of awards: majority of awards to north east coast (NY, Pennsylvania), west coast (CA) and southern states (TX, FL). There is a good balance in participation of groups that are underrepresented in science and engineering: Women have slightly higher numbers of awards, and the percentage for URMs changes significantly, increasing over the years.

There is a reasonable balance in awards to different types of institutions: large majority are to Research Intensive PhD Institutions; a very small number are to PUI, but this is also a result of the low number of proposals received from PUI.

## **OTHER TOPICS**

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.

A high percentage of proposals go to research intensive institutions, and a very small percentage going to PUIs. The program has not funded 2-year institutions/community colleges. Perhaps the program could find ways to encourage this community to get involved in this research.

While the COV is aware that this consequence as unintentional, the COV views the one proposal per cycle policy, combined with the slow turnaround time, as a particular difficult situation for new investigators who often need multiple attempts to be successful with their first proposal.

Some COV members recommend that the NSF carefully evaluates the effects of the single proposal per year policy, for example, allow investigators without current NSF funding to submit more than one proposal.

2. Please provide comments as appropriate on the program's performance in meeting programspecific goals and objectives that are not covered by the above questions.

The program has developed a good balance between established and new career investigators.

Similarly, there is generally good balance in geographical distribution of awards. However, the COV members in the break out group wondered how these fared when considering how many proposals were submitted per geographical region.

Well balanced portfolio, addressing NSF mission and priorities. Good number of co-funded proposals with other programs and across divisions. This speaks of an excellent program that does well at finding opportunities with partnering programs.

For early career investigators, the mentoring resources that NSF has should be better advertised and accessible, for example creating an early career webpage with links to the resources.

3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

Having a spreadsheet of all potential reviewers and ranking based on their historical reviews helps POs find best suitable reviewers. Extending award duration to four or five years would be very helpful. Current cycle limits outcomes and forces PIs to write renewals on year two, mid cycle in their grant period. Feedback from reviewers could be provided in a more timely manner. Currently, feedback is provided only a couple of months before the next round of proposals is due.

The COV recommends that PIs be encouraged to contact program officers to discuss proposal submissions. This could avoid situations where highly ranked proposals are not funded due to issues other than merit review.

4. Please provide comments on any other issues the COV feels are relevant.

All programs could benefit from requesting more support for online education and research activities. In a situation like COVID, these have become critical and could benefit NSF funded efforts and programs. The COV template could be streamlined to help members answer the most relevant questions to each program.

Some COV members feel that an alternative mechanism to the one proposal per year will benefit the research community. They appreciate the open aspect of submitting a full unsolicited proposal, and the emphasis on single PI proposals because this is complimentary to other funding agencies. However, some COV members will like more submission opportunities than once a year. For example, a shorter proposal with a shorter turnaround time that could provide faster feedback to early career investigators.

5. NSF would appreciate your comments on how to improve the COV review process, format and report template.

COV report could be done every five years, rather than the shorter cycle used at present. Having access to full list of reviews/reviewers, as well as whom among these were in panel vs. ad-hoc reviews, as well as their funding and review history, would be helpful to COV members. The COV believes that one account to login will be helpful.

## INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

## **REU/SP - Research Experiences for Undergraduates and Special Projects**

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

#### I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?	
Comments: REU: Reviews were conducted by panel, which is valuable for calibrating people to the expectation level appropriate for an REU. These would not have been appropriate by ad hoc review.	REU: yes SP: yes
SP: Special project reviews were conducted by staff, which was the most appropriate. These seemed to be implemented appropriately.	
Data Source: EIS/Type of Review Module	
2. Are both merit review criteria addressed	REU: mostly
a) In individual reviews? REU: Usually. SP: Yes.	SP: yes
b) In panel summaries? REU: Yes. SP normally does not have panels.	
c) In Program Officer review analyses? REU: Yes. SP: Yes.	
Both of the criteria were addressed well in the special projects portion of the review, and were very consistently addressed.	

In the REU reviews, there doesn't seem to be consistency in the definition,	
evaluation, and weighting of the intellectual merit criterion verses the broader	1
impacts. Calibration of reviewers and appropriate communication of the	1
weighting of these objectives should be improved. We would recommend:	1
<ol> <li>Create clear definitions for these in the scope of an REU program,</li> </ol>	1
acknowledging that there will be overlap for the categories of intellectual	
merit and broader impact.	1
<ol><li>Clearly communicate definitions to the PI and reviewers, prior to</li></ol>	
commencing review of proposals.	1
3) Create a concise definition of intellectual merit within the context of an	1
REU experience for students in a single term.	1
<ol><li>Provide all panelists with a copy of the solicitation prior to commencing</li></ol>	1
review, which outlines the criteria, including as it relates to program	
structure.	1
Data Source: Jackets	

3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	REU: sometimes
<b>REU</b> : Sometimes. However, there are examples where the individual reviewers written reviews differ from the panel summaries. This was very inconsistent for individual reviewers. Different reviewers emphasized completely different aspects of merit (publications vs. recruiting vs. professional development).	SP: yes
Reviewers should continue to be encouraged to make sure their final reviews reflect the panel summary. It is often difficult to understand why a particular proposal was ranked a certain way. It may be that the difficulty reviewers face is that REU has a tendency to be all things to all people, and the guidelines are broad enough that it is difficult for reviewers to write a succinct explanation on why a particular proposal really stands out relative to other proposals. A clearer understanding on the goals of the program would help guide reviewers and make it easier for proposers to understand the ratings for their proposals.	
We recommend that it should be made clear to all reviewers to be more thorough in assessing both intellectual merit and broader impact aspects of the review, as well as how those relate to program structure.	
SP: Reviews are largely internal. However, see comments under Question 5.	
Data Source: Jackets	
4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	REU: Mixed
REU: Summaries reflected what the reviewers said, but it didn't fill in the gaps present from individual reviews. These summaries should have helped to	SP: N/A

provide additional detail and give a comprehensive view of the two impact criteria. For many of the proposals (those funded) the panel summaries were very useful and informative.	
SP: N/A	
Data Source: Jackets	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	REU: yes SP: Not always
<b>REU</b> : While the rationale is provided, it is sometimes still a little puzzling why the deficiencies found in one REU site proposal are not considered to be as problematic as similar deficiencies found in another REU proposal.	amayo
Better clarity is needed on what is funded and what is not, specifically in the Review Analysis	
The documentation for the rationale was reflected in the PO comments. The individuals providing this should be commended for their efforts here, especially since they often are filling in large gaps from individual reviewers.	
<b>SP</b> : Sometimes the internal reviews are quite critical, yet the proposal was funded anyway.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	REU: usually SP: yes
REU: Documentation is very good, states why the proposal was funded or declined. One slight problem is that when the panel changes its mind on a proposal during the meeting, they often do not change their written individual reviews to reflect any changes in their thinking as a result of the panel discussion. Better clarity is needed on what is funded and what is not (in Review Analysis) Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
<ul> <li><b>REUs</b>:</li> <li>1. Many of the reviews need significant proofreading and editing. This should be required of reviewers as part of their panel work.</li> </ul>	

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- 2. If the mission of the program was better clarified, it would make it easier for reviewers to be more effective using the merit review process. We recommend that more clear definitions are put in place for the two different criteria (intellectual merit and broader impact), with appropriate calibration for what should be expected of an REU.
- 3. Based upon reviewer comments, there seems to be a general belief among people who propose REU programs (at R1s), and in many cases the reviewers, that PUIs generally offer no research or poor-quality research and the only real opportunities for research are the PhD-granting R1 institutions. This is often not the case. In some parts of the country and types of institutions research opportunities for undergrads tend to be limited at R1 institutions, while MS-granting and 4-year universities can have vibrant research programs with lots of research opportunities for undergrads specifically (all year round, not just in the summer). Perhaps there should be some instruction about this in the guidelines; the presumption of poor research opportunities at non-R1s paints an inaccurate picture, which can impact the significance of the proposal (especially the recruitment plans).
- 4. Some reviews provide the negative criticism that a proposed REU program is "traditional". What is necessarily wrong with that? Wouldn't "tried and true" be a benefit when we are trying to train and excite students? Isn't it more likely that the students will have a bad outcome with a creativesounding but untested plan (which could go very badly)? Even if ultimately the "traditional" criticism did not make it into the PO's review analysis as a reason to suggest a decline of the proposal, it is still seen in the panel summary. This could give PIs the impression that they need to include something really "out there" for their next try, which is not necessarily going to be for the benefit of the students. This relates back to #2 (above).
- 5. Is it realistic to expect extensive numbers of publications based on work done by undergraduate students over the course of 10 weeks in the summer? Some of the reviewers are especially critical about the lack of publications from the REU programs (that are submitting renewals or who had REU programs in the past). There should certainly be expectations that students present posters of their work or give talks.
  - Is there any investigation done to find out whether REU students listed on publications actually provided substantive contributions to the work? Or are they added to inflate the numbers of publications that can be reported? *Perhaps the annual reports should require a brief description of what each REU student contributed to each publication.*
- Better metrics for assessing proposal ideas about recruiting and student pools and better metrics for assessing the outcomes on renewals would be useful. It is clear that tracking students after they leave the REU experience would be a better metric for determining if the program is effective.
**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	REU: yes SP: yes
The program did a very good job of selecting a diverse panel of reviewers (underrepresented groups, gender, institutional size), including a strong representation from PUIs.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	REU: yes SP: yes
Standard COI procedures appear to work well in this case, from what we could assess in the provided information.	
Data Source: Jackets	
3. Additional comments on reviewer selection: We applaud and encourage NSF's efforts to have as diverse a pool of reviewers as possible.	
We recommend that more appropriate calibration for what should be expected of an REU, particularly as it relates to the intellectual merit and broader impact, along with how to best incorporate evaluation of a program/site.	

# **III. Questions concerning the management of the program under review**. Please comment on the following:

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

The Program Officers are to be commended for their dedication to their work, their responsiveness to PIs, and their efforts to distribute NSF funds widely and fairly. For REU, workloads for NSF program officers, PIs, and reviewers would be reduced with a more clearly defined mission statement.

The program demonstrates a diversity of target groups (underrepresented groups, gender, institutional size, and geography) and schools represented, including international programs.

2. Responsiveness of the program to emerging research and education opportunities.

**REU:** It seems that the program is aware of the evolution of some of the "best practices" for REU sites, but should also be careful about getting charmed by the newest ideas at the detriment of practices that are known to work.

The program is very responsive to providing a variety of experiential learning opportunities to the students. A number of programs incorporated site visits to companies in the chemical enterprise.

**SPECIAL PROJECTS**: It is unclear how many proposals are invited, or are in response to inquiries. The question that cannot be answered here is: what are they targeting for invited proposals?

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

**REU**: In many cases, the prioritization across a set of proposals was unclear. The distinction between proposals that were funded and not funded were not apparent, based on the panel summaries and the review analysis.

**SP:** Collaboration between program officers and submitters of special projects proposals was very evident in the submissions, which were well thought out.

4. Responsiveness of program to previous COV comments and recommendations.

**REU**: The concerns about the lack of scientific merit review in previous reviewer comments have been resolved. There was a good response to moving the REU program reviews to panels, which are more appropriate.

Some reviewers still seem to need additional review training in order to provide appropriate, sufficient meaningful quantities of feedback as it relates to both intellectual merit and broader impact, which was a noted issue from the 2016 COV. There are still issues with some reviewers being too brief with their reviews, which do not provide sufficient constructive feedback to the PI submitting the proposal.

Clarity still needs to be provided to both PI's and reviewers as to whether or not the research of the REU students' needs to be centered around a single theme, or if a broader survey of areas is appropriate.

There are still inconsistencies in what is intellectual merit vs. broader impact within the scope of an REU program, acknowledging that there will be overlap for these categories.

**IV. Questions about Portfolio.** Please answer the following about the portfolio of awards made by the program under review.

### 1. Balance across disciplines:

• In general, REU topics fall in general areas of chemistry, biochemistry, modeling, and materials, which is representative of the domains that fall under chemistry. Many REU proposals are collaborations within a department. Thus, there is appropriate balance across disciplines.

### 2. Award size and duration

• REU: size and duration are similar (except for international sites)

### 3. Awards to new- and early-career investigators

- REU: success rate similar to success rates overall.
- PROJECTS: it is rare to see new PIs or co-PIs on these (mostly invited) proposals.

### 4. Geographical distribution

- There is a remarkable lack of REU sites in California, which not only has a very large population, but also has a very large population of URM students.
- There is a limited number of REU programs in the central part of the country.
- Special Projects were largely east coast centric.

# 5. Awards to different types of institutions

• REU: Very few proposals from institutions with MS as the terminal degree are awarded REUs. Is there a reviewer bias above that these types of institutions are not believed to have good-quality research or quality opportunities.

# 6. Innovative and potentially transformative projects

• Not really applicable to these programs

# 7. Inter- and multidisciplinary projects

• REU: a significant number of interdisciplinary projects or themes are REU sites.

# 8. Projects that integrate research and education

• By their nature, REU inherently integrate research, education, and opportunity.

# 9. Participation of groups underrepresented in STEM

It is clear that a major focus of the REU and Special Projects is to provide otherwise unavailable opportunities to underrepresented students. This is a major commitment especially in the REU program. SPECIAL PROJECTS:

- Although the internal reviewers do look at the proposed invitees to some of these workshops and try to ensure there is demographic and geographic representation, as well as some involvement with PUIs, the lists they finally approve are sometimes still have very nominal inclusion in some categories. Perhaps there should be a requirement of some more expanded access to the workshop than just invitees? This would be consistent with NSF policies of access.
- Requirements for invitees to workshops should not just be that there are attendees from underrepresented groups; there should be a consideration of representatives from HBCUs and other minority-serving institutions (*no matter what their color*) who will represent the needs of these diverse groups of students / researchers.

### 10. Projects that are relevant to agency mission or national priorities

• By definition, the entire REU program fits with the NSF mission to broaden participation in STEM, particularly by underrepresented groups.

# **OTHER TOPICS**

- 1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.
- We feel that the philosophy and goals of the REU program need to be clarified. The program feels like the wild west, where different proposals can be rated highly, or poorly, without clarity of what a particular program stands out. This dilemma seems to stem from the fact that most Ph.D. REU sites have their first goal to recruit graduate students to their program. Is this in fact the first, and most important, goal of the REU program? Another goal is to increase the research opportunities for students who do not have access to research at their home institutions. These goals align when diverse students do not have opportunities at their home institutions, and diverge when they have plentiful research opportunities. Some state systems, for example, have copious undergraduate research opportunities available outside of the most research-intensive universities. Clarification of the goals of the program would help focus reviewer's attention on the most important elements of the recruitment and assessment plans. Once NSF has clarity on the goals of the REU program, they can re-write the RFP.
- A second point is that if NSF could provide guidelines for assessment, that would also help focus the review process. Since a main goal of the program is to retain more students in STEM careers, then programs should track their students through their careers for as long as they have funding from NSF. (For instance, Linked In could be used to track students over time.) Renewals should favor those programs that have done the best job of providing research experiences to a diverse group of students (women, students of color, low socioeconomic status, students with disabilities, first generation, etc.) and helping propel them to careers in STEM.
- Finally, we believe that the entire REU program needs to be evaluated longitudinally to understand what has worked, and what is missing, in the context of deciding on any revision to the program guidelines.
- 5. NSF would appreciate your comments on how to improve the COV review process, format and report template.
  - Provide more guidance to help COV participants by providing a checklist and sequence of activities to get them started.
    - Tell people to read the previous report.
    - Provide the template immediately

# INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

# **SYN:** Chemical Synthesis

Briefly discuss and provide comments for *each* relevant aspect of the program's review process and management. Comments should be based on a review of proposal actions (awards, declinations, returns without review, and withdrawals) that were *completed within the past four fiscal years*. Provide comments for *each* program being reviewed and for those questions that are relevant to the program(s) under review. Quantitative information may be required for some questions. Constructive comments noting areas in need of improvement are encouraged.

# I. Questions about the quality and effectiveness of the program's use of merit

**review process.** Please answer the following questions about the effectiveness of the merit review process and provide comments or concerns in the space below the question.

QUALITY AND EFFECTIVENESS OF MERIT REVIEW PROCESS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
<ol> <li>Are the review methods (for example, panel, ad hoc, site visits) appropriate?</li> <li>The review methods are appropriate. The merit review process was utilized well for this program. All proposals were reviewed by least three reviewers through either the panel or mail-in process. The panel reviews were often supplemented with ad-hoc reviews for needed subject matter expertise and to give new reviewers some experience through panel participation. For those reviewed by panels, 601/656 (91.6%) proposals received panel summaries. The Panel Summaries help PIs understand the basis for an award decision.</li> <li>The COV perceives a shift towards a higher fraction of panel reviews (away from ad hoc reviews) in the past 4 years. While ad hoc reviewers tend to have more closely aligned expertise, their scoring is less well-calibrated. Scores may also be higher because ad hoc reviewers cannot compare the quality of different proposals or rank them. PIs can suggest ad hoc reviewers but panels probably have few PI-suggested reviews (probably 1 or 0, and very hard to get more given the numbers). This could give an advantage to proposals that only have mail-in reviews. We wonder if scores from mail in and panel reviews really should be averaged together, as they seem to be.</li> <li>In addition, the panel discussion can be a valuable part of the assessment, particularly when reviewers have very different views of a proposal. The discussion can bring to light information that reviewers may have overlooked, and includes the views of panelists who were not assigned to review. The evolution of reviewer solutions after discussion was evident in the panel summaries and program officer notes in several jackets.</li> </ol>	YES, and trending in a good direction

The decision of a program officer who has only ad hoc reviews can seem arbitrary when it requires weighting divergent reviews. Ad hoc reviews may also focus more on PI reputation and past accomplishments, apply inappropriate criteria, or make inappropriate comments (such comments are probably self- redacted during panel reviews). The challenge with panel reviews is the lower overall level of expertise for any particular proposal, which leads to some reviews being overly generic or uncritical. A proposal whose area does not fit well in the panel to which it is assigned may not resonate well with the panel members, and be unfairly disadvantaged. Some SYN proposals that were more focused on applications such as catalysis may have suffered from this. The addition of ad hoc reviewers to panel reviews as needed where proposals do not have enough expertise is encouraged.	
Given the breadth of the SYN program, a portion of the proposals fall outside the review panel sub-disciplines. These proposals were reviewed exclusively by a mail-in process. Such mail-in reviews were important, as the process provided a larger pool of reviewers with broader expertise. In cases of mail-in only reviews, it is important that the PI receives detailed PO comments. The decision to handle some proposals entirely by ad hoc review needs to be well-justified. Explanations like 'too few proposals' or 'not a good fit' may have merit but did not seem like imperatives to the COV, on the basis of the information provided and our view of the proposal topics. Some proposals (EAGER) appropriately received only internal reviews. These reviews tend to be brief and focused on technical issues. <b>Data Source: EIS/Type of Review Module</b>	
2. Are both merit review criteria addressed?	
a) In individual reviews?	YES
b) In panel summaries?	YES
c) In Program Officer review analyses?	YES
Both criteria are generally addressed by reviewers and in panel summaries. Templates do help and uniformity is increasing. The COV is concerned that some reviewers do not use standard criteria, for example, commenting on	
historical impact vs. current activities.	

There is some confusion among reviewers about the distinction between broader impact (significance, applications) and intellectual merit. In some cases, it can be a gray area.	
Reviewers may also discount participation in institutional outreach vs creating one's own activities, and whether training activities must be innovative. There is inconsistency in how to judge leveraging.	
Sometimes the program officer adjudicates after the fact, but for general misconceptions it would be better if the clarification were provided during the panel discussion?	
Reviews of accomplishment-based proposals may not provide enough information about broader impacts, focusing primarily on intellectual merit. However, our sample size is small and may not be representative.	
Data Source: Jackets	

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3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?	YES, mostly
Many reviews are very substantive and carefully weigh both criteria in explaining their final score, although the more substantive comments in the reviews were typically directed at the intellectual merits. The vast majority of reviews were consistent with letter rankings. In a few instances, the letter rankings did not seem to match the critiques. More guidance to reviewers about the ratings might help with this issue.	
However, the COV noted that the quality of the reviews is variable and some are considerably more substantive than others. The problem is not only the lack of information but also that some proposals are penalized if the review is not substantive.	
Some reviewers incorrectly conflate PI prestige (without pointing to specific accomplishments) with proposal quality. Some reviewers judge the merit of a project on recent past productivity, counting papers without taking into account differences in styles and effort. Scoring should primarily focus on the proposed work.	
Reviewers do not always take into account how far the NSF funds can be expected to go, and how much the funds are supplemented by other resources, in judging productivity. Some reviewers incorrectly conflate synergistic activities with broader impacts. Some reviewers express their enthusiasm by inappropriately making funding recommendations in their review.	
Data Source: Jackets	

4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?	YES, mostly
The use of panel summary templates has been beneficial in terms of standardizing content and language. Nevertheless, there are still examples of panel summaries that inappropriately recommend proposals for funding, and may need more guidance from the program officer.	
A few summaries were not well-aligned with panel reviews. In some cases, this may be a natural consequence of panel discussion. However, in other cases the panel summary seems unduly dominated by a particular review (often, a highly critical one).	
Data Source: Jackets	
5. Does the documentation in the jacket provide the rationale for the award/decline decision?	YES
The rationale for the award/decline decision was provided by the review analysis. It is a very helpful document, providing a clear and detailed explanation for why each decision was made. The review analysis also showed how the discussions in panels helped to converge towards a consensus. Some review analyses included suggestions to the PIs to improve their proposals.	
The COV saw instances of program officers whose justification for discounting advice of the panel was not convincing. More justification should be supplied in these cases.	
The consultation between several program officers to come to a decision on a borderline proposal is a good practice and is strongly encouraged. The COV would like to know more about the mechanism by which this consultation takes place, and how the division encourages it.	
Analysis of other funding in the making of an award is done thoroughly and is commended.	
Data Source: Jackets	

6. Does the documentation to the PI provide the rationale for the award/decline decision?	PARTLY
Reviews, panel summaries, and PO comments were provided to the PIs typically around the same time. These, together, give a very good rationale for the award/decline decisions.	
Some program officer comments are very brief. For the declined proposals, providing more constructive feedback drawn from the review analysis into the	

PO comments would help PIs with future submissions. For reviews by mail-in reviews only, it is important that the PO comments contain sufficient information regarding the basis for the funding decision. Phone conversations with PIs could be documented better.	
The division's outreach to the community on the meaning of "broader impacts" has been helpful.	
The COV saw one instance of a very well-reviewed proposal that was declined based on the panel discussion. To provide constructive feedback to the PI, it is important to share how the proposal fared in the panel discussions and recommendation, even if only in general terms. Overall, proposals that received high ratings but do not fare well in the discussion should be explained more carefully in the panel summary.	
Data Source: Jackets	
7. Additional comments on the quality and effectiveness of the program's use of merit review process:	
The use of accomplishment-based proposals should be reconsidered – they are based on past achievements, not forward-looking research directions, and are harder to review fairly.	

**II. Questions concerning the selection of reviewers.** Please answer the following questions about the selection of reviewers and provide comments or concerns in the space below the question.

SELECTION OF REVIEWERS	YES, NO, DATA NOT AVAILABLE, or NOT APPLICABLE
1. Did the program make use of reviewers having appropriate expertise and/or qualifications?	YES
The POs did a very good job handling the review processes in an efficient manner. The discussion of the proposals demonstrates that the reviewer expertise was sufficient, and that the panels provided a great platform for sharing expertise. For proposals that did not well fit a particular panel, some mail-in reviews provided a very good means for evaluation, as the SYN program covers a large, diverse array of chemical syntheses.	
The participation of reviewers from PUIs (specifically for RUI proposals), industry, and women is needed, and the program should ensure that it continues to include them as appropriate.	
GOALI proposals should try to have more industry participation in the review to help reviewers and program officers to better understand what industry is likely to disclose.	
Supplementing panel review with additional ad hoc review can add expertise. However, it does not seem to be done consistently, and averaging scores of panel and ad hoc reviewers may not be appropriate.	
Data Source: Jackets	
2. Did the program recognize and resolve conflicts of interest when appropriate?	YES
handled COIs well. Panelists having a conflict-of-interest with a specific proposal did not review that proposal and exited from the meeting during the discussion.	
Data Source: Jackets	
3. Additional comments on reviewer selection:	

# **III.** Questions concerning the management of the program under review. Please comment on the following:

# MANAGEMENT OF THE PROGRAM UNDER REVIEW

1. Management of the program.

Overall, the program was managed very well. Many panels addressed a wide range of sub-topic areas, and the proposals were reviewed in accordance with the two criteria of intellectual merit and broader impacts. Given the tight funding, PIs of funded proposals were sometimes asked to reduce their budgets. While most reductions were handled well, the reductions, in some cases, led to a substantial shrinkage in funding for undergraduate research.

The low submission rate of proposals by women PIs is a concern, which was noted to be below the Division average. To address this may require more outreach/encouragement by the POs.

2. Responsiveness of the program to emerging research and education opportunities.

The program has responded well to emerging research and education opportunities. Several proposals were jointly funded with the SusChem initiatives. Panels for Synthetic Methods and Organometallic research ensured that new advances could be pursued in organic and inorganic chemistry. The COV particularly appreciated the support for interactions with industry (in student training) and community colleges (for broader impacts). Reviewers are in general appropriately cognizant of emerging opportunities in research.

The COV saw one instance of a program officer making a decision to fund a borderline proposal that was deemed too risky by the panel due to a lack of preliminary results, and another of a program officer funding a proposal that drew sharply divergent reviews by the EAGER mechanism. The latter is a worthwhile approach to initiating new areas.

The identification of 'hot' areas can become a self-fulfilling prophecy, where areas are 'hot' because they are well-funded (and therefore generate a lot of proposals, high impact journal publications, and citations).

It is not clear to the COV that emerging education opportunities are a priority for the program. The program should consider making emerging broader impacts (not just education) a funding priority, a current example being COVID-19 research.

3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.

This SYN program is largely curiosity-driven and multidisciplinary. The research portfolio appears to be balanced. If a particular portfolio is emphasized, more explanation would help understand the decision. Program officers appear to try to fund more risky research, and avoid double dipping.

It is not clear how proposals are grouped, sizes of group, and decisions about how many to fund in each group. Information about how funding priorities are determined between panels/groups of proposals could be helpful in understanding the prioritization process.

# 4. Responsiveness of program to previous COV comments and recommendations.

The program shows good direction in terms of transparency and justifying funding decisions, especially proposals that are declined. However, some of the program officer comments communicated to the PI seem very brief in some of the more controversial declines. Later comments (2019) seem more complete than earlier ones (2016).

The program has invited junior faculty from declined grants in the proposal review and panels, providing these young investigators an opportunity to learn the review process and improve their own proposal grantsmanship. Perhaps these could be addressed further, which one could anticipate would improve the funding ratio for 1<sup>st</sup>-time investigator grants. It also is suggested that efforts be taken to improve to the funding of female PIs and proposals from small institutions.

	Name	Affiliation
COV Chair or	Dr. Peter Dorhout	Kansas State University
Co-Chairs:	Dr. Robert (Bob) Cave	Harvey Mudd College
	Dr. Malika Jeffries-EL	Boston University
MPS Advisory	Dr. William (Bill) Tolman	Washington University - St. Louis
Committee Liaison		
COV Members:	Dr. Jose Almirall	Florida International University
	Dr. Mario Alpuche	University of Nevada - Reno
	Dr. Lane Baker	Indiana University
	Dr. Lisa Berreau	Utah State University
	Dr. Lionel Cheruzel	San Jose State University
	Dr. Ya-Huei (Cathy) Chin	University of Toronto
	Dr. Carlos Crespo-Hernandez	Case Western Reserve University
	Dr. Karin Crowhurst	California State University - Northridge
	Dr. Rick Danheiser	Massachusetts Institute of Technology
	Dr. Krishna Foster	California State University - Los Angeles
	Dr. Matthew Francis	University of California - Berkeley
	Dr. Marcelo Guzman	University of Kentucky
	Dr. Gene Hall	Rutgers University - Piscataway
	Dr. Aaron Hieb	Genentec
	Dr. Timothy Jackson	University of Kansas
	Dr. Kayunta Johnson-Winters	University of Texas - Arlington
	Dr. Daniela Kohen	Carleton College
	Dr. Johna Leddy	University of Iowa
	Dr. Yi Liu	Lawrence Berkeley National Laboratory
	Dr. Samantha MacMillan	Cornell University
	Dr. Psaras McGrier	Ohio State University
	Dr. Adam Myers	SSCI
	Dr. Kristin Omberg	Pacific Northwest National Laboratory
	Dr. Mary Jo Ondrechen	Northeastern University
	Dr. Elizabeth Papish	University of Alabama - Tuscaloosa
	Dr. Mark Pederson	University of Texas - El Paso
	Dr. George Schatz	Northwestern University
	Dr. Susannah Scott	University of California - Santa Barbara
	Dr. George Shields	Furman University
	Dr. Mary Jane Shultz	Tufts University
	Dr. Joseph (Joe) Subotnik	University of Pennsylvania
	Dr. Marilyn Tourne	Tuskegee University
	Dr. Sergei Iretiak	Los Alamos National Laboratory
	Dr. Javier Vela	Iowa State University
	Dr. Maria Vicente	Louisiana State University
	Dr. Lauren webb	University of Texas - Austin
	Dr. Anna wenzel	Viaremont Nickenna College
Dr. Lewis whitehead Nimbus Therapeutics		Nimous Inerapeutics
	Dr. Ziling (Ben) Xue	University of Tennessee - Knoxville
	Dr. Rebecca Zangmeister	National Institute of Standards and Technology

# Appendix A: List of Members of the 2020 COV

# Appendix B: Charge to the COV

# Charge to the FY 2020 Chemistry Division (CHE) COV December 12, 2019

By NSF policy, each program that awards grants and cooperative agreements must be reviewed at four-year intervals by a Committee of Visitors (COV) comprising qualified external experts. NSF relies on their judgment to maintain high standards of program management, to provide advice for continuous improvement of NSF performance, and to ensure openness to the research and education community served by the Foundation. Reports generated by COVs are used in assessing agency progress in order to meet government-wide performance reporting requirements.

Decisions to award or decline proposals are ultimately based on the judgement of NSF staff informed by evaluations from qualified reviewers who reflect the breadth and diversity of the proposed activities and the community. Systematic examination by the COV of a wide range of funding decisions provides an independent mechanism for monitoring and evaluating the overall quality of the Division's decisions on proposals; program management and processes; and the resulting portfolio.

The FY 2020 Division of Chemistry (CHE) COV is charged to address and prepare a report on:

- the Division's response to the prior COV report of 2016;
- the integrity and efficacy of procedures implemented to solicit and review proposals, and processes used to recommend and document proposal actions;
- the quality and significance of the results of the Division's programmatic investments;
- the relationship between the portfolio and the Missions of the Division, the Directorate, and the Foundation; and
- the Division's engagement in, and prioritization of, research initiatives.

The review will assess operations of individual programs in the Chemistry Division (CHE) for four fiscal years: FY 2016-2019. The CHE programs under review include:

- Chemical Catalysis (CAT)
- Chemistry of Life Processes (CLP)
- Chemical Measurement and Imaging (CMI)
- Chemical Structure, Dynamics, and Mechanisms- A and B (CSDM- A and B)
- Chemical Theory, Models and Computational Methods (CTMC)
- Environmental Chemical Sciences (ECS)
- Macromolecular, Supramolecular and Nanochemistry (MSN)
- Chemical Synthesis (SYN)
- Centers for Chemical Innovation (CCI)
- Research Instrumentation Program and Facilities (MRI and facilities)
- Research Experiences for Undergraduates Sites (REU)
- Special Projects and Initiative Investments

# Appendix C: Breakout Groups

Program	Program Round 1 Assignments			
САТ	Ya-Huei (Cathy) Chin	Psaras McGrier	Elizabeth Papish	Anna Wenzel
CCI	George Schatz	Mary Jane Shultz	Javier Vela	
CLP	Lionel Cheruzel	Aaron Hieb	Kayunta Johnson-Winters	Mary Jo Ondrechen
CMI	Jose Almirall	Lane Baker	Rebecca Zangmeister	
CSDM-A	Mark Pederson	Daniela Kohen	Carlos Crespo-Hernandez	
CSDM-B	Timothy Jackson	Maria Vicente	Ziling (Ben) Xue	
СТМС	Joseph Subotnik	Lewis Whitehead	Sergei Tretiak	
ECS	Marcelo Guzman	Krishna Foster	Kristin Omberg	
MRI	Marilyn Tourne	Lisa Berreau	Gene Hall	Samantha MacMillan
MSN	Mario Alpuche	Yi Liu	Lauren Webb	Matthew Francis
<b>REU/SP</b>	George Shields	Johna Leddy	Karin Crowhurst	
SYN	Susannah Scott	Rick Danheiser	Adam Myers	

# First Program Review (Leaders (Scribes) in Blue)

# Second Program Review (Leaders (Scribes) in Blue)

Program	Program Round 2 Assignments				
CAT	Daniela Kohen	Lionel Cheruzel	Susannah Scott	Yi Liu	
CCI	Krishna Foster	Mario Alpuche	Rebecca Zangmeister	Aaron Hieb	
CLP	Matthew Francis	Elizabeth Papish	Carlos Crespo-Hernandez	Lewis Whitehead	
CMI	Kristin Omberg	Marcelo Guzman	Mary Jane Shultz		
CSDM-A	Johna Leddy	Lauren Webb	Joseph Subotnik		
CSDM-B	Lisa Berreau	Rick Danheiser	Sergei Tretiak		
CTMC	<b>Mary Jo Ondrechen</b>	George Schatz	Mark Pederson		
ECS	Gene Hall	George Shields	Samantha MacMillan		
MRI	Karin Crowhurst	Jose Almirall	Lane Baker		
MSN	Javier Vela	Maria Vicente	Ya-Huei (Cathy) Chin	Marilyn Tourne	
REU/SP	Adam Myers	Timothy Jackson	Kayunta Johnson-Winters		
SYN	Ziling (Ben) Xue	Psaras McGrier	Anna Wenzel		

# Appendix D: Agenda

#### Agenda Division of Chemistry Directorate for Mathematical and Physical Sciences 2020 Committee of Visitors

#### All Times are Eastern Daylight Savings Time.

### Sunday, May 31, 2020 (Optional – Open to all COV Members)

- 7:00 8:00 PM Informal Gathering Time with Chairs
- 8:00 9:00 PM Zoom Break-out Group Practice

### Monday, June 1, 2020

- 10:00 AM Welcome and Charge to the Committee of Visitors MPS Acting Assistant Director, Mathematical and Physical Sciences (MPS) – Sean L Jones
   CHE Division Director – David Berkowitz
   COV Chairs – Drs. Peter Dorhout, Malika Jeffries-EL, Robert (Bob) Cave
- 10:30 AM FACA / Conflict of Interest Briefing MPS Staff Associate - Kathy McCloud
- 10:45 AM Break (10:45 11:00 AM)
- 11:00 AM First Program Review Round 1 Break-Outs (Program Staff to join for first ~15 minutes, then will be available for questions via phone or email)
- 12:30 PM Break (12:30 1:30 PM)
- 1:30 PM Prepare First Program Review Report
- 4:00 PM First Program Review (Draft) Due to Chairs / Break (4:00 4:30 PM)
- 4:30 PM Second Program Review Round 2 Break-Outs (Program Staff to join for ~15 minutes, then will be available for questions via phone or email)
- 6:00 PM Adjourn for Day

#### Tuesday, June 2, 2020

10:00 AM Discussion of First Program Review (ALL)

- 10:30 AM Prepare Second Program Review Draft
- 11:30 PM Second Program Review (Draft) Due to Chairs / Break (11:30 12:30 pm)
- 12:30 PM Merge First and Second Program Review
- 2:00 PM Merged Program Review Due to Chairs / Break (2:00 3:00 PM)
- 3:00 PM Chairs' Comments Merged Program Review
- 3:30 PM Consideration of Portfolio Questions- Round 1 (COV members choose group)
- 4:45 PM Portfolio Responses Round 1 Draft Due To Chairs / Break (4:45 5:00 PM)
- 5:00 PM Consideration of Portfolio Questions Round 2 (COV members choose group)
- 6:30 PM Portfolio Responses Round 2 Draft Due to Chairs / Adjourn

#### Wednesday, June 3, 2020

- 10:00 AM Gathering
- 10:15 AM Merge Reports Portfolio Questions
- 11:30 AM Submit Merged Portfolio Questions to Chairs / Break (11:30-12:30 PM)
- 12:30 PM Discussion of Final Report: Writing and Preparation of Presentation
- 1:45 PM Working Session for Chairs / Break (1:45 PM 2:00 PM)
- 2:00 PM Final Questions to CHE
- 2:30 PM Complete Final Report and Presentation
- 4:00-5:30 PM Report to Acting AD and Division of Chemistry
- 5:30 PM Adjourn

# Appendix E: Division Wide Statistics for the COV

# NSF COMMITTEES OF VISITORS (COVs)

The table below was completed by program staff.

Date of COV: June 1-3, 2020

Program/Cluster/Section: All programs in CHE

**Division:** Chemistry

**Directorate:** Mathematical and Physical Sciences

**Number of actions reviewed:** 354 (337 projects, 17 collaboratively linked) + 9 Preliminary CCI

Awards: 146 (143 projects)

**Declinations:** 199 (185 projects)

Other: Invited: 3 (3 projects); Not Invited: 6 (6 projects); Other: 9 (9 projects)

Total number of actions within Program/Cluster/Division during period under review:

Awards: 2001 (1887 projects)

**Declinations:** 4659 (4362 projects)

Other: Invited: 53 (53 projects); Not Invited: 165 (165 projects); Other: 80 (76 projects)

# Manner in which reviewed actions were selected:

A spreadsheet was created of the 6,755 competitive actions (6,338 distinct actions and 417 non-lead linked collaboratives) ascribed by the NSF database to the Chemistry Division in FY 2016 - FY 2019. FY attribution is based on the date action was completed, rather than on the submission date. In most instances, the two are the same; exceptions are proposals submitted in a September window (the Federal FY starts October 1) and CAREER proposals (which are generally received in July of FY [N-1] and processed in FY [N]). A separate spreadsheet was generated for the 218 CCI preliminary proposals.

Data retrieved for each proposal included the FY, proposal number, PI, senior personnel, institution, managing program and program officer, targeted program announcement (or not), collaborative status (lead, non-lead, or not a collaborative), outcome (award,

declination) and reviewer/panelist names. A random number generator was then used to place the proposals in a completely random order.

A grid was created for each of the reviewed programs, containing as columns the four FY being reviewed and as rows the types of actions (clear and marginal awards and declinations) and major types of proposals (CAREER, RUI). Proposals were drawn from the top of the randomized list to fill the slots on the grid, skipping entries for which there were institutional or individual conflicts of interest with COV members. Single proposals were also drawn from the top (where available) for major initiatives, for EAGERs, and for Accomplishment-Based Renewals. Finally, the grids were checked to ensure that each program officer actively engaged in the program was represented; additional proposal(s) were drawn from the top of the list as needed to assure this representation. To avoid duplication or overrepresentation, only the leads of collaboratively linked proposals were considered. For each program, one proposal (only) returned without review during the COV period (80 proposals, including 15 non-leads) was selected from the top of the randomized list.

Because of the small number of proposals involved, the Centers for Chemical Innovation program was treated differently. All proposals managed in this program were screened for conflicts of interest with COV members. Those Phase 2 proposals without conflicts with the subset of members assigned to this program were put forward, along with one award and two declinations, plus one invited and two not invited preliminary proposals (all selected in sequence from the top of the randomized lists, excluding identified conflicts of interest) for each Phase 1 competition.

For the Instrumentation program, clear and marginal awards and declinations were included for proposals under \$1 M from PhD-granting (249) and Primarily Undergraduate (286) institutions and for proposals over \$1M (20). These categories were treated separately in the NSF-wide competition. The only unconflicted midscale proposal was also selected. This process resulted in selection of 346 proposals total, or roughly 5% of the pool. 17 of these (~5%) were leads of collaboratively linked proposals, roughly matching the representation of collaboratives (~5%) in the pool.

A few additional proposals were added (after screening for conflicts of interest) in response to specific requests during the meeting. Access was blocked for proposals where a COV member had a COI identified either before or during the onsite COV meeting.

# Appendix F: Portfolio Questions

**Q1:** The quality and significance of the results of the Division's programmatic investments. As you look at the awards in EJacket, please consider the Annual and Final Project Reports and Project Outcomes. Consider the Products (books, journal or juried conference papers, patents, thesis/dissertations) that have been produced as a result of the research as well as the Participants/Organizations that have been involved in and/or trained during the project. Please read through the Impacts sections to consider the impacts on chemistry and on other disciplines, also on the development of human resources, infrastructure, technology transfer, in addition to the impacts on society beyond science and engineering. Note: many of the awards that you will review are on-going, so the "impact and significance" may be a work in progress. Also, not all awards will involve all categories of impact.

See also: <u>News – Chemistry (CHE)</u> for recent news stories highlighting CHE awards.

**Q2:** The relationship between the portfolio and the Missions of the Division, the Directorate, and the Foundation. Please consider the initiatives that NSF, the Directorate of Mathematical and Physical Sciences (MPS), and the Division of Chemistry have had during the COV period (FY 2016-2019). Is CHE's participation in the various initiatives appropriate in terms scope and level of participation? Are there NSF and MPS initiatives that CHE should have participated in and didn't?

For information that may help in answer this portfolio question, please see NSF CHE's website on <u>Active Funding Opportunities</u>, <u>Chemistry's new Solicitations and Cross-Agency Program</u> <u>Descriptions</u>, and <u>Chemistry's Dear Colleague Letters (DCL)</u>. For a list of Selected CHE Solicitations, Dear Colleague Letters, Supplement Opportunities, etc. also see p.30 of the COV CHE Divisional Presentation:

- NSF's 10 Big Ideas: Quantum Leap, Understanding the Rules of Life, Harnessing the Data Revolution, Mid-Scale Research Infrastructure
- Understanding the Brain
- Sustainable Chemistry, Engineering and Materials (SusChEM); Innovations at the Nexus of Food, Energy and Water Systems (INFEWS); and Critical Aspects of Sustainability (CAS)
- Computation and Data-Enabled Science and Engineering (CDS&E)
- o International Supplements in Chemistry
- Non-Academic Research Internships for Graduate Students (INTERN)

Q3: The Division's engagement in, and prioritization of, research initiatives.

Consider the Division's engagement with the community via Chemistry Newsletters, Workshops, Town Hall Meetings, Conferences, etc. Does the Division do a good job in engaging all stakeholders? If no, how could the interactions be improved? Are new initiatives broadly advertised and adequately described? Does the Division receive sufficient input from the community on prioritizing research initiatives and their funding levels?

For some helpful links, see: <u>CHE Newsletters and Workshop Reports</u>, Chemistry Blogs on Tumblr

# Appendix G: Members of the Portfolio Question Discussion Groups

Assignments of COV Members to Portfolio Questions for the two discussion sessions.

COV Members	Session 1 Question	Session 2 Question
Almirall, Jose	1	3
Alpuche, Mario	3	1
Baker, Lane Allen	1	2
Berreau, Lisa	1	2
Cheruzel, Lionel	1	2
Chin, Cathy	1	2
Crespo-Hernandez, Carlos	3	1
Crowhurst, Karin	1	2
Danheiser, Rick	2	3
Foster, Krishna	3	1
Francis, Matthew	1	2
Guzman, Marcelo	2	1
Hall, Gene	2	3
Hieb, Aaron	1	2
Jackson, Timothy	3	1
Johnson-Winters, Kayunta	1	2
Kohen, Daniela	1	3
Leddy, Johna	2	3
Liu, Yi	2	3
MacMillian, Samantha	1	3
McGrier, Psaras	3	1
Myers, Adam	1	2
Omberg, Kristin	2	3
Ondrechen, Mary Jo	3	1
Papish, Elizabeth	1	2
Pederson, Mark	1	2
Schatz, George	2	1
Scott, Susannah	1	2
Shields, George	1	3
Shultz, Mary Jane	2	1
Subotnik, Joseph	1	3
Tourne, Marilyn	3	1
Tretiak, Sergei	1	2
Vela-Becerra, Javier	1	3
Vicente, Maria	1	3
Webb, Lauren	1	3
Wenzel, Anna	2	1
Whitehead, Lewis	2	3
Xue, Ziling	2	3
Zangmeister, Rebecca	2	3
Cave, Robert (Chair)	3	3
Dorhout, Peter (Chair)	1	1
Jeffries-EL, Malika (Chair)	2	2
Tolman, Bill (MPS Liaison)		

# Appendix H: Portfolio Question Responses

# Q1: The quality and significance of the results of the Division's programmatic investments.

As you look at the awards in eJacket, please consider the Annual and Final Project Reports and Project Outcomes. Consider the Products (books, journal or juried conference papers, patents, thesis/dissertations) that have been produced as a result of the research as well as the Participants/Organizations that have been involved in and/or trained during the project. Please read through the Impacts sections to consider the impacts on chemistry and on other disciplines, also on the development of human resources, infrastructure, technology transfer, in addition to the impacts on society beyond science and engineering. Note: many of the awards that you will review are on-going, so the "impact and significance" may be a work in progress. Also, not all awards will involve all categories of impact.

### See also: <u>News – Chemistry (CHE)</u> for recent news stories highlighting CHE awards.

Generally, from the eJackets provided, the Products, Participants/Organizations, and impact on chemistry and other disciplines was well described. From the reports, the Chemistry Division is clearly engaged in research and education that is high in intellectual merit and has significant broader impacts in society and education. As the central science, research in the Chemistry Division portfolio was observed to clearly touch other programs in MPS, the NSF and society. Members of the COV committee noticed that some reports gave very little information about the progress of the research. It was noted that some initial reports submitted for the first time were returned so that more information could be provided. For many projects evaluated, the research is a work-in-progress, and many are early in the grant cycle. Annual highlights are effective tools for scientific communication but are underutilized.

Another concern was that most of the reports focused more on intellectual merit and less on broader impacts. This made it difficult to measure/determine the impact on society and the proposed outreach efforts. Therefore, NSF should recommend that this section be populated with concrete examples of how these efforts are being pursed, and institute more mechanisms for accountability. Many members suggested that the NSF could include the number graduate /undergraduate students and collaborators that work on the grant as a metric to help assess the broader impacts.

Several members of the COV did commend the CCI program for producing quality research that resulted in high profile publications. However, several members noted that excellence is not all about publishing papers in high impact journals, and the NSF could do a better job at publicizing the major accomplishments of this program (and others) to the general public.

In addition, the discussion largely evolved into how we define goals, metrics, and success at both the level of an individual award and at the broader program/division level. Extracting quantitative data for the program and even for an individual proposal in the present format is difficult; qualitative data can be extracted more readily, but at a significant cost in terms of time/effort. This led to further discussion on reporting and how reporting could be improved or

used more effectively. Specifically, for responding to the COV, getting standardized data on products for the COV would help making this assessment – perhaps major deficiencies would be more obvious and help make this aspect a data driven process.

Listed below are some specific suggestions that might lead to better reporting for individual awards were also discussed. These include:

- Showing relevance of a PI and a research lab/program over a longer timescale might prove merit and impact more effectively for fundamental research. This could be captured in the NSF biosketches.
- A minimum set of criteria (papers and/or publications and/or students trained) might be useful in clarifying expectations and identifying potential areas of concern early. Criteria may be flexible depending on the research area and award mechanism.
- Annual highlights (which are already requested) are effective but underutilized.
- PIs are trained extensively in grant writing and in proposal preparation. Project reporting is not taught as effectively and there might be value in training.
- An idea of surveying participants in the award beyond the PI (e.g. longitudinal studies of students, postdocs, and outreach participants) could have value in establishing impact and effectiveness. Ways to collect reliable data on mentoring, building the STEM workforce and broader impacts have room for improvement. Note this idea was not a consensus opinion agreed on by all panel members, primarily stemming concern in burdens of reporting.
- Multiple COV members expressed aversion to the present annual report form length, complexity, uncertainty in what is most important that make it hard from the PI perspective to know what constitutes a good annual report. Individual project reports might be flexible according to the project.
- An NSF report detailing the progress of the graduate/undergraduate students and overall impact of the entire body of work after the final report is submitted would also be useful for assessing the significance of the work (additional longitudinal tracking).
- Many members noted that publications after the final report is submitted are not always included. The PI could be allowed to submit this information, or it could be submitted by the host institution. The NSF could remind PIs beyond the grant's life-cycle.

**Q2**: The relationship between the portfolio and the Missions of the Division, the Directorate, and the Foundation. Please consider the initiatives that NSF, the Directorate of Mathematical and Physical Sciences (MPS), and the Division of Chemistry have had during the COV period (FY 2016-2019). Is CHE's participation in the various initiatives appropriate in terms scope and level of participation? Are there NSF and MPS initiatives that CHE should have participated in and didn't?

For information that may help in answer this portfolio question, please see NSF CHE's website on Active Funding Opportunities, Chemistry's new Solicitations and Cross-Agency Program Descriptions, and Chemistry's Dear Colleague Letters (DCL). For a list of Selected CHE Solicitations, Dear Colleague Letters, Supplement Opportunities, etc. also see p.30 of the COV CHE Divisional Presentation:

- NSF's 10 Big Ideas: Quantum Leap, Understanding the Rules of Life, Harnessing the Data Revolution, Mid-Scale Research Infrastructure
- Understanding the Brain
- Sustainable Chemistry, Engineering and Materials (SusChEM); Innovations at the Nexus of Food, Energy and Water Systems (INFEWS); and Critical Aspects of Sustainability (CAS)
- *Computation and Data-Enabled Science and Engineering (CDS&E)*
- International Supplements in Chemistry
- Non-Academic Research Internships for Graduate Students (INTERN)

Point 1. New Initiatives and Investment. Chemistry is present in many of these initiatives, but the COV would like to encourage greater participation in these programs, as this has the capacity to bring additional funds to the CHE division. This being said, it should be emphasized that there should be a balance between fundamental and applied science, and that the primary mission of CHE should remain to explore PI-initiated, curiosity-driven proposals. The COV would like to know (1) how does NSF define these initiatives and 10 Big Ideas and (2) for whom these initiatives are being prioritized and defined for? The committee felt that it was important to focus on the overall mission of fundamental science and emphasized that participation in specialized programs should be prioritized for this. Representatives from each subfield could cite instances within their COV dockets that involved solicitation to these programs. It was found that some directives mapped easily onto CHE. Others are very distinct and a stretch to connect to CHE. The committee found that proposals that capitalized on these programs were of good quality.

Point 2. The COV believes that, through these initiatives, the Chemistry Division could bring in additional resources. However, a stronger linkage between the individual chemistry disciplines to the bigger initiatives is needed. It would be helpful for NSF to organize workshops far in advance and to help PIs on aligning their work to these big initiatives. The COV has the impression that, in selected cases, the information on the specific calls, the proposal evaluation mechanism, and even the background of the proposal reviewers to the interdisciplinary work are relatively unclear. These aspects could be made more transparent.

The COV feels that these initiatives, if well planned and promoted, are a vehicle to bring in more resources into and to excite the field, bringing more awareness on chemistry related topics. For example, Quantum Leap had been a success in nucleating research activity in the field. The panel

would like an assessment of the outcomes of these initiatives, specifically on (i) the success stories, (ii) which universities and/or other institutions have benefitted, and (iii) the funding rates for proposals that are associated with these initiatives.

Point 3. Balance between "New" Initiatives and Existing Programs. The COV emphasizes that there must be a balance between the investment of research funds into both the new initiatives and existing programs. These should be a parity in portfolio investments between the latest, more trendy work, and the core, fundamental areas of chemistry. Despite this, we encourage the division to pursue these initiatives in areas that have overlap, as these initiatives have the ability to enhance the CHE funding.

Point 4. How do these Initiatives Promote the Broader Impact? The COV cautions that the initiatives, if not managed well, may actually limit the broader impact, because of the confined research scope; therefore, it is critically important to understand who defines and identifies these initiatives? How do we, as chemists, have a greater voice in defining the scientific road map and ensuring that the investment of research fund is well made?

It is noted that the international supplement to the research activity supporting trainees to perform or participate research work abroad is a highly valuable experience for the trainees. CHE had invested  $\sim 600$  K per year through the International supplement program to support research activities in  $\sim 30$  countries. A newer, INTERNS supplement, is currently at the initiation phase and has a lower participation. COV anticipates an increase in participation to this new supplement.

Point 5. Initiative Participation by CHE. The CHE division has been active in promoting opportunities regarding the science mission of the division, the directorate, and the Foundation. The NSF Acting Division Director has been prolific in "Dear colleague" letters to inform the chemistry community of opportunities. Currently, these letters are directed to current and previous PIs; COV encourages the broader distribution of these letters, to collaborators, potential new PIs, and those in the industry. The CHE division has held workshops and office hours regarding initiative information sessions. Many of these have been moved online due to the recent COVID-19 pandemic. Attendance at these online sessions appears to be good. The committee felt that this could be a cost-effective mechanism for informing the CHE community that should be continued. In addition to workshops, social media (e.g., Twitter, LinkedIn) could be helpful in promoting CHE participation in specialized opportunities.

# Q3: The Division's engagement in, and prioritization of, research initiatives.

Consider the Division's engagement with the community via Chemistry Newsletters, Workshops, Town Hall Meetings, Conferences, etc. Does the Division do a good job in engaging all stakeholders? If no, how could the interactions be improved? Are new initiatives broadly advertised and adequately described? Does the Division receive sufficient input from the community on prioritizing research initiatives and their funding levels?

#### **Responses:**

\* The Division does a good job of reaching out to the community in a number of ways, and the Division is encouraged to streamline the information sent to PIs. There is a lot of information that PIs get inundated with – is there a way to streamline this? One way to do this would be to have Program Officers send correspondence to investigators associated with their specific program. The COV members recommend that the Division continue sending regular newsletters because they are useful to the community. All of the data regarding workshops, reports, and newsletters should be on the website. Some of the COV members noted that the latest posted newsletter is from summer 2018. While there are more recent newsletters, some COV members had trouble finding/accessing them, and the COV recommends that the division continue to update their website to reflect new information in a timely manner. The COV recommends that CHE reach out to a broader the pool of people with these current methods (e.g. newsletters). For industry, national labs and other funding agencies, there is a bit of lag with respect to communication – some of the stakeholders had never seen the newsletters, for example, and it would be good to come up with some ways to reach these stakeholders and disseminate the information.

\* The COV members encourage the Division to better reach out to junior faculty. The COV members believe that when the Division focuses on junior faculty, it also enables broadening participation because junior faculty hires tend to be more inclusive and diverse. One possibility is creation of a new faculty portal where junior or early career faculty sign in and get added to the reviewer database.

\* Some schools have senior faculty that help younger colleagues navigate grants systems or workshops to get more information/feedback, however, without these, do junior faculty know how to access and contact the Division? Junior faculty are usually overwhelmed with information. Hence, the COV members think that the Division should encourage and reach out to senior faculty and chairs of departments to direct and mentor junior faculty to the various NSF opportunities. Sending NSF information to the chairs of departments may be a more effective communication platform to reach the junior faculty than broad emails to all faculty community already in the Division's list.

\* The Division is encouraged to continue inviting junior faculty in panel reviews. A junior faculty member can greatly benefit from participating in panels with more experienced faculty members, learning how the reviewing process is done and what is expected from a successful grant proposal. Moreover, new faculty contribute to the review process by bringing a fresh perspective and focused area of expertise. In-person panels are also an excellent networking opportunity. Members of the COV also highlighted that seniority does not necessarily equal enhanced reviewing skills. In the invitation to young panelists, there should be an explicit statement about how useful the panel will be to improving their future proposals. Nevertheless, they should also be reminded that saying "no" will not impact future grant proposals. It is important to survey new investigators, including those with significant social burdens, before assuming the in-person review does not accommodate their needs. The Division should consider using hybrid panel reviews (in-person and virtual) more broadly to increase diversity and to better accommodate junior faculty with many other responsibilities.

\* The COV also recommends that the Division includes more workshops targeting junior faculty and underrepresented communities. At smaller colleges and universities, although there is good research, faculty members rarely apply for CAREER awards and there seems to be a missed opportunity for these stakeholders. It seems that the Division has not figured out how to better support these stakeholders that do not have institutional support for grant writing workshops, etc.

\* The Division should strive to make the information more widely available, particularly reaching out more aggressively to underrepresented minorities and underserved communities. New diversity initiatives should be supported by the Division that promote diversity and inclusion including a good plan for sustainability and accountability. Members of the COV questioned whether the Division is doing enough in reaching out to underserved communities such as through the American Indian Science and Engineering Society (AISES), the National Organization of Black Chemists and Chemical Engineers (NOBCChE), the Society for the Advancement of Chicanos and Native Americans in Science (SACNAS) and other science diversity organizations. The Division needs to show up at the national conferences of these organization.

\* In this regard, the Division should initiate new programs (successors to previously successful programs) to increase diversity and inclusion. It was emphasized that a single project or program will not fix the systemic problem of the lack of diversity; these problems are far from solved and the Division needs to do more. Calls for new proposals to support diversity and inclusion would be strengthened by requiring a robust plan for sustainability after the grant has expired.

\* The Division should consider adding and/or emphasizing inclusion and diversity into the program announcements and adding communication in the program announcements targeting underrepresented groups.

\* The Division is encouraged to continuing supporting programs that are doing important work, such as REU and diversity and inclusion programs. If a program is addressing an unsolved problem and is successful, it may be no longer innovative but still necessary. Programs should continuously be funded when they have a track record of doing great work at mentoring undergraduate students without the added pressure of innovation in their operation, or when training students and researchers, because the research thrusts are innovating. The COV members questioned why change something when it is working. Although the Division values innovation when forming a program, best practices in existing in REU and diversity and inclusion programs should be continued.

\* PIs get emails from the division at a good pace, information dense and helpful – opportunities to meet POs at conferences, funding sources – can quickly see the content that is relevant to them.

\* Can there be a formalization between the NSF and other organizations (ex. ACS) to raise awareness of these interactions? An idea would be for NSF PO members to attend governance committees on the Saturday prior to the national convention, or even become formal members of divisions like ORGN, MEDI, COMP, ANYL etc. \* Early career workshops are known and there is an afternoon at national ACS conferences for questions/training. It would be interesting to see what the attendance of these events at ACS are. People can sign up for a time to meet one-on-one with POs and other people at NSF. The system is there, it's possible that it's not convenient for people—great way for people who did come to ask if the program they wanted to submit to was appropriate, but it's possible that people just don't go for whatever reason.

\* Having headquarters NSF staff visit colleges and universities is also a possibility (and has been done before) and works really well for in-person "office hours."

\* In the last 2-3 months, the division has virtual office hours to engage the community and announce new programs, answer questions. This was implemented for COVID-19 restrictions, but is a useful meeting that is open to stakeholders and the COV recommends that these virtual office hours should continue.

\* Social media is necessary for reaching younger stakeholders. There is a generic NSF site for Twitter, in particular, but it would be useful to have one that is CHE specific. Not having a presence on social media represents a huge missed opportunity for the division.

\* There are few applications from PUIs, 2-year, 4-year institutions—these stakeholders may not frequent national meetings. The Division should increase its effort at reaching out to these institutions to get additional proposals submitted. If there is the opportunity to speak to colleagues that haven't been exposed to the possibilities for funding, etc., then there might be more submissions. The committee is concerned that funding is not distributed equitably throughout the country. More deliberate communications with industrial partners and institutions of higher learning in under-represented states of SBIR and GOALI funding opportunities is merited.

\* Wild idea? Mercury and Associations of PUI professors – help faculty develop proposals, rich vibrant community. The Division is encouraged to create such a coalition for different chemistry groups to be able to communicate. Ex: shared clusters for computational chemists, etc.

\* A general way that information gets out to PUIs is CUR (Council on Undergraduate Research) – they do workshops on how to get funding, they invite faculty and write chairs of departments (Dreyfus, NSF, NIH, Research Corp) and provide mentors. The Division should consider partnering with this program to improve involvement.

\* The Division is encouraged to reach out to pre-doctoral students and doctoral students and engage in getting more individual applications from these students, such that by the time they become faculty, they have some experience in writing grants. Engage younger students earlier in writing grants to NSF. Gives them good preparation about who to talk to and where to go to for information and NSF then will get more applications from young faculty.

\* Vehicle to interact with young faculty in particular – Gordon conferences are excellent opportunities to really have an opportunity to speak informally especially with junior faculty. In order to do this, there should be funding available for each PO to attend at least one of these

Gordon conferences each year. NSF should not limit travel funds as these conferences are a missed opportunity to cultivate new opportunities and getting to know young researchers and new chemistry. The COV recognizes that NSF is trying to put all funds toward research and it is not possible for NSF staff to receive outside funding for travel, but COV members think travel to conferences, especially intimate gatherings like the Gordon conferences, by POs would be important to support the overall mission of NSF and drum up new proposals for stellar science. The COV notes that there are stark differences between funding agencies in this regard: DOE/DOD all show up to every conference, they learn who is doing exciting stuff, and are available to talk. NSF is almost completely absent from these meetings.

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For the Division of Chemistry Committee of Visitors Dr. Peter K. Dorhout Chair