

**Report of the 2016 Committee of Visitors
Division of Chemistry
National Science Foundation**

**Meeting Dates
May 11-12, 2016**

**Submitted on behalf of the Committee by
Sharon Hammes-Schiffer, Chair**

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CCI: Centers for Chemical Innovation	33
CLP: Chemistry of Life Processes	42
CMI: Chemical Measurement and Imaging	51
CSDM-A: Chemical Structure, Dynamics and Mechanisms A	60
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CTMC: Chemical Theory, Models and Computational Methods	76
ECS: Environmental Chemical Sciences	84
EDU: Educational Activities	93
INSTR: Major Chemical Research Instrumentation and Facilities	107
MSN: Macromolecular, Supramolecular and Nanochemistry	116
SYN: Chemical Synthesis	124

I. Executive Summary

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.

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.

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.

II. Background

The Committee of Visitors (COV) for the Division of Chemistry (CHE) met for two days to review the activities of the Division during the three-year period 2013-2015. The meeting was held on May 11-12, 2016. Appendix A provides a list of the membership of the committee, whose 27 members include the COV Chair, Dr. Sharon Hammes-Schiffer, and a liaison from the Directorate for Mathematical and Physical Sciences (MPS) Advisory Committee, Dr. Graham Cooks, as well as a number of prominent chemists from academia, industry, government laboratories, and other federal agencies.

The COV was charged to address and prepare a report on:

- The quality and effectiveness of the merit review process;
- The selection of reviewers;
- The management of the programs under review;
- The management of the overall portfolio including the balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators.

In early April 2016, prior to the meeting of the COV, a video teleconference was conducted to prepare the COV members for the review process. This teleconference was conducted by the CHE Division Director, Dr. Angela Wilson, the MPS Staff Associate, Dr. Eduardo Misawa, and several others from the CHE Division. The COV members were given a presentation on conflicts of interest and confidentiality, a short 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 2013 COV report and the CHE responses to it over a three-year period. After the main teleconference, 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 May 11, 2016 with a welcome by Drs. Wilson and Hammes-Schiffer. These remarks were followed by a short briefing on conflicts of interest (COIs) by Dr. Misawa. The charge was officially presented to the COV by Dr. Fleming Crim, Assistant Director of the Directorate for Mathematical and Physical Sciences. The letter stating the formal charge appears in Appendix B of this report.

After the completion of the formalities, the COV members were separated into twelve groups representing the different areas of CHE. The CHE programs that were reviewed included:

- CAT: Chemical Catalysis
- CMI: Chemical Measurement and Imaging
- CTMC: Chemical Theory, Models and Computational Methods
- CSDM-A: Chemical Structure, Dynamics and Mechanisms A
- CSDM-B: Chemical Structure, Dynamics and Mechanisms B
- CLP: Chemistry of Life Processes
- EDU: Research Experiences for Undergraduates Program and other Educational Special Activities
- ECS: Environmental Chemical Sciences

- INSTR: Major Chemical Research Instrumentation and Facilities
- MSN: Macromolecular, Supramolecular and Nanochemistry
- SYN: Chemical Synthesis
- CCI: Centers for Chemical Innovation

Each group or subpanel was provided with access to a selected number of proposal “jackets”. The jackets were selected to represent a number of clearly fundable cases, clear declinations, and a larger fraction 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 morning subpanel according to their primary sub-discipline of chemistry. Each member was also assigned to an afternoon 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 a closed session for two hours over a working lunch and for one hour at the end of the afternoon of the first day to discuss the general recommendations and themes emerging from the subpanels. The morning of the second day was spent preparing merged reports by the combined membership of the first and second round subpanels and preparing the global draft report. During this time, the CHE Division Director and Deputy Division Director were available to answer questions from the committee.

The remainder of the second day was devoted to preparing the draft report, beginning with a closed session with only the COV members present in the room in order to encourage frank discussion among the members. In the afternoon, the COV Chair presented the COV’s findings and recommendations to the MPS AD, the Deputy Division Director, the Division Director, and the Program Officers. The MPS AD met with the COV after the presentation for further discussion about the findings and recommendations.

The membership of the subpanels and the complete agenda for the meeting are provided in Appendices C and D, respectively. The final merged reports for each of the subpanels are included in Appendix E.

Explanatory note: The data herein is reported by the members of the COV. The Chemistry Division provided the COV with data from NSF’s Enterprise Information System. Data is sensitive to the formulation of queries and may not necessarily be directly comparable to that from other NSF sources.

III. Specific Results of the Review

A. Integrity and Efficacy of Processes

1. Review Process

Overall efficacy of review process

Overall, the COV was impressed with the quality and efficacy of the merit review process. The Program Officers play a crucial role in overseeing the review process, and the COV

commends their efforts. In general, the COV found that the Program Officers selected reviewers with appropriate scientific expertise, while maintaining diverse representation from reviewers at different career stages, at different types of institutions, and of both genders. To ensure appropriate alignment with the scientific objectives of the CHE Division, the COV recommends that the majority of reviewers hold active research positions in the chemical sciences. The COV also recommends that the Program Officers continue efforts to curate a database of competent reviewers and avoid soliciting reviews from individuals with a history of providing poor quality or unsubstantiated reviews.

The majority of programs review proposals using a combination of in-person and virtual panels. The scientific expertise of the panel is augmented by soliciting mail-in ad hoc reviewers as necessary. This practice was viewed positively by the COV, and the Program Officers are encouraged to rely on the panel review process when possible. The use of virtual panels can help recruit reviewers who may be reluctant to travel to an in-person panel, thereby serving as an avenue to achieve appropriate expertise and diversity. A significant advantage of panels is that the Program Officers are able to effectively remind the reviewers of the review criteria, particularly the consideration of broader impacts. Another advantage is the opportunity for discussion of divergent reviews.

The COV was impressed with the level of detail and justification for award/decline decisions contained within the Program Officer's Review Analysis document. However, the amount of information from the Review Analysis that is shared with the PIs in written form varies among the Program Officers. As the Program Officers represent a critical line of communication between the program and the PIs, the COV recommends that the Program Officers provide appropriate elements of the Review Analysis, in writing, to the PIs. Although the COV recognizes that certain confidential information must be redacted, access to the remaining information is particularly important for PIs with declined proposals, as the details in the Review Analysis can help inform the PI with respect to resubmission.

Effective and consistent utilization of panels

Although most programs use panels, some of them still rely solely on mail-in reviews or do not utilize the panels as effectively as possible. The COV recommends that panels be used consistently, augmented by mail-in reviews as appropriate. The panel members should be selected carefully to cover the scientific topics of the proposals, as well as to include researchers from both PUIs and PhD granting institutions. The Program Officers should also strive to optimize the effectiveness of the panels by giving clear instructions at the start of the meeting, ensuring that all panel members feel free to speak freely, and encouraging reviewers to change their scores and reviews after the panel discussion if warranted. To prevent individual reviewers from consistently ranking too high or too low, the Program Officers should instruct panelists to use the full range of rankings for all proposals being reviewed and to perform a preliminary ranking of the proposals at the start of the meeting. The Program Officers should also clarify the definition of broader impacts and the metrics for assessment and weighting at the start of the meeting to ensure consistency. Moreover, while most panels usually contain broad representation, it is important for the Program Officers to guide the discussion, as needed, to account for and

value the broad representation of the PIs and grants reviewed. Although in-house panels are considered to be more effective, virtual panels are more attractive to qualified reviewers whose other commitments make travel difficult. However, the virtual panels should be strongly directed by the Program Officer to maintain the focus of the reviewers.

Clarification of the assessment, weighting, and accountability of the broader impacts

Although the Division has made substantial effort to clarify the definition of broader impacts and to explain how they will be assessed and weighted, confusion in the community still remains. The Program Officers should clearly explain to both the mail-in reviewers and the panel reviewers how the broader impacts should be assessed and weighted. The PIs should also be held accountable for completing the proposed broader impact activities and should be required to provide an explanation if certain portions were not completed or were replaced by alternative activities. The Program Officers should check that the annual progress reports reflect progress on the broader impacts described in the proposal. In addition, the reviewers should be instructed to evaluate the broader impacts as well as the research from the previous grant cycle. Accountability is necessary to ensure that PIs propose realistic broader impact activities and to ensure that the community benefits from the completion of these activities.

2. Selection of Reviewers

The COV commends the Division and the Program Officers for what is a tremendous effort to obtain reviews from reviewers with appropriate expertise in a timely manner, and to assemble panels that need to reflect not only expertise in the area of the proposals being reviewed, but also a balance in gender, URM, types of institutions, and career stages of the panelists. This effort is greatly complicated by the need to consider conflicts of interest and other constraints that prevent people from participating as panelists or reviewers.

To maintain and improve the quality and timeliness of the review process and panel discussions, the Division should continue using the reviewer database as a source for appropriate reviewers with necessary expertise. In addition to data on how often reviewers have served, this database should include information on the timeliness of the responses from the reviewer, participation of the reviewer in panels, and average rankings provided by the reviewer. For additional expertise, the Program Officers should consider using publications databases, such as ISI Web of Knowledge, to find experts who are currently publishing in the area. Finally, to further assist the Program Officers in selecting reviewers and in managing conflicts of interest, the Program Officers should encourage PIs to make more frequent use of the ‘List of Suggested Reviewers and Reviewers not to Include’. The general perception in the community seems to be that inclusion of this list is detrimental to the review of the proposal, and this perception should be dispelled.

3. Program Management

The Program Officers are key to the success of the scientific programs. Their responsibilities span from very high levels in terms of identifying frontier research areas, balancing portfolios, and advocating for increased resources, to more routine tasks of

identifying reviewers, organizing panels, and writing review analyses. Their workload is high, yet their performance in managing the review process is admirable and should be commended. They have the authority and latitude to make decisions based on the recommendations of the ad hoc reviews and the panel. As such, the Program Officer role is one that requires great dedication, integrity, and leadership.

Effectiveness and continuity of program officers

The Program Officers need to be knowledgeable about current topics and issues in the field. They also need to be able to select qualified reviewers, convene effective panels, and interpret the reviews in a manner that ensures well-balanced and fair decisions. The Program Officers were uniformly excellent in managing conflicts of interest, balancing portfolios, and including a mix of PUI and PhD institutions in the review process. The COV identified that strong leadership was critical for the success of panels, both virtual and in-person, in the review process. Not all Program Officers were equally effective in this role, particularly in communicating the collective analysis from the panel to the PI, and the COV noticed substantial variability in the quality of the panel reviews and summaries sent to the PI. Of more concern was that some final decisions seemed incommensurate with the ad hoc and panel reviews and were not thoroughly justified in the Review Analysis.

Clearly, successful program management requires a diverse skillset and often involves a high workload for the Program Officer. As such, the COV recommends that for programs led by a single Program Officer, a strategy and contingency plan be in place in the event that the Program Officer is unable to perform her/his responsibilities. At the very minimum, a rotator or back-up Program Officer should be assigned and cross-trained to ensure that proposals continue to be handled efficiently and fairly.

The COV appreciates the value of a mix of experienced permanent Program Officers and rotators who bring expertise and fresh perspective from the community. The 2013 COV report expressed concern that rotators, while often effective, had not built the relationships within NSF to support cross/inter-disciplinary projects. The current COV feels that the value of excellent rotators outweighs this concern. Ideally, rotators would serve a three-year term, with overlap staggered among rotators so that the administrative learning curve is spread among years. New rotators should be paired with experienced Program Officers.

Transparent communication of basis for decision to decline

There is a perception in some parts of the chemistry community that the determination of funding decisions lacks rigorous analysis and at times seems arbitrary, resulting in low confidence in the NSF review process by these researchers. While the COV was very impressed with the depth and critical thought of the Review Analyses, the Program Officer Comments transmitted to the PI on declined proposals were brief and often less informative. Although PIs are encouraged to call the Program Officer, often the calls do not occur or important information concerning declinations is not conveyed effectively by phone. The COV feels that more transparent communication to the PI on declined proposals is critical and that as much of the Review Analysis as possible should be made available to the PI in written form. It is understandable that information that compromises

the identity of reviewers or other PIs cannot be provided. The COV notes that the NSF Proposals and Award Policies and Procedures Guide, Part I, Section G indicates that the PI can request and obtain any releasable material in the file on his/her proposal.

4. Resulting Portfolio

The COV firmly believes that the primary focus of the CHE Division should center on supporting fundamental research and encouraging transformative science. We commend the division on its lean administrative operations and relatively low non-research expenditures. This level of expenditures on items other than research is similar to highly rated, large non-profit grant foundations and has allowed NSF to spend ~90% of its budget on fundamental scientific research during the years 2013-2015. Overall, the COV feels that the Division is doing an excellent job deploying the vast majority of its resources to research grants in an essentially flat budget environment. However, the average number of proposals per Program Officer has increased significantly over the last ten years. If proposal growth continues as it has over the past decade, the number of Program Officers will need to increase to maintain the high quality of the review process and the research that is funded.

The COV feels strongly that the ~26% proposal funding rate leaves a significant number of excellent proposals unfunded. However, increasing funding rates with a flat budget for the Division would reduce individual grant sizes. Many existing grants already have had their budgets reduced compared to the requested amount, with the result that the nation will not receive the full impact of the proposal. Thus, reducing grant sizes further to allow a higher funding rate would be counterproductive and is not recommended. We therefore advocate an increase in total funding to the NSF Chemistry Division to increase the impact of chemistry on innovation in the United States and thereby to offer a long-term competitive advantage to this country. In the absence of such an increase in total funding, we recommend that the Division maintain or preferably increase the size of the individual grants, even if the result is to slightly decrease the funding rate.

The distribution of funds among individual investigator awards appears to be mostly driven by the number of proposals received. In other words, the community has significant control over the portfolio weightings by virtue of the proposal topics submitted. The COV feels that this approach is desirable for NSF, which should not limit the scope of science funded, in contrast to other more mission-driven agencies. The awarded proposals are of high quality in their respective programs, which also reflects an overall balanced portfolio across the Chemistry Division. The geographic distribution of awards is consistent with national demographics and population densities, while some heterogeneity among individual programs exists. Although occasionally in certain programs, COV members noted an imbalance in award distribution, overall the percentages for funding among different institution types and underrepresented groups seems appropriate.

Supporting fundamental research and transformative science

The COV strongly recommends that the primary focus of the Division centers on

supporting fundamental research and encouraging transformative science. At times, these funds are diverted to new programs or initiatives. Instead of diverting funds from fundamental research, the COV suggests that the Division minimize such new programs unless additional funds are secured. Moreover, the grant size is often too small to enable the PIs to pursue transformative science and instead leads to more conservative research. Increasing the grant size will enable the PIs to pursue exploratory research in new directions, leading to greater innovation and higher potential for transformative science. The COV recommends increasing the grant size for proposals that appear to be particularly innovative or transformative in intellectual merit.

Broadening participation

Many efforts to increase inclusiveness in the chemical enterprise have not taken into consideration the vast differences between two-year and four-year PUIs or even the significant variability among four-year PUIs. Some four-year PUIs have a rich history in receiving funding from the Chemistry Division through the mentoring of their PIs in the art of funding acquisition as well as the presence of significant resources on their campus to support research, while others do not have these advantages. The same situation is found for PhD granting institutions. The top 100 PhD granting programs in the country receive the majority of funding in several Chemistry Division programs, thereby limiting the diversity of thought and perspective contributed to the programs of the Division. Additionally, this situation limits the availability of training opportunities to only select institutions.

Many programs have been developed over the years to increase the submission of proposals from URM and women in chemistry. These efforts have involved outreach to specific types of institutions and workshops that provide instruction without much follow up. As many URM and women in academia do not populate the institutions where a history of funding from the NSF is a strong part of the culture, it is vital that opportunities are created to allow for a progressive pathway for creating this culture. The availability of mentored research grants, for which a senior investigator agrees to serve as a mentor, at the assistant professor and mid-career level would be a reasonable means by which to accomplish this goal. Such mentorship could take place across institutions if needed. The grants would be associated with the development of relationships and networks needed to sustain research funding over long periods and to subsequently allow these new PIs to transmit their experiences to other members of their departments and institutions, creating a culture of funding.

Importantly, the Division should hold both individual and larger programs accountable for outcomes from activities aimed at inclusion. A focus on the influence of implicit bias in review processes is needed to reach these goals.

B. Performance in Contributing to Strategic Goals of Division and Foundation

The performance in contributing to the strategic goals of the Chemistry Division and the Foundation is exemplary, as described by the following analysis of research, education, and instrumentation. A careful assessment of the effectiveness of the Centers of Chemical

Innovation (CCIs) and a continued strengthening of collaborations with international and industrial partners are recommended.

Maintaining focus on core mission of fundamental research in chemistry

Estimated data from the Chemistry Division indicate that the Division is a lean organization, in which the vast majority of the budget goes to support basic research, as opposed to education, outreach, and workforce development. To put these numbers in the usual context, estimated overhead rates are on the order of 7%. However, there are undoubtedly additional overhead expenses associated with NSF funded activities that are not represented in the formal budgets. For example, the various Centers perform administrative tasks within each Center, including administering internal competitions for Center funds and financial management. Even allowing for these costs, it is reasonable to estimate that 90% of the Chemistry Division budget goes to fundamental research.

Given the Chemistry Division's 90% expenditure on fundamental research, any significant decrease in the Division's funding would be unfortunate. However, such a decrease has not been observed. This analysis suggests that fundamental research in chemistry is indeed being well-protected by the Foundation. The COV commends the Division for focusing the funding primarily on fundamental research and strongly encourages the continuation of this practice.

Centers of Chemical Innovation

The CCI program is unique within the Chemistry Division and warrants special consideration. CCIs are an opportunity to demonstrate that chemistry, often referred to as the central science, can indeed be central to large research efforts that span aspects of engineering, the environment, and medicine in both academic and industrial venues. The centers enable chemists to take on grand challenges that cannot be addressed by individual investigators or even individual institutions. When they succeed, the discoveries of the centers can be inspirational and provide innovation that can drive new basic science and applications beyond the center itself. The synergy should extend to educational opportunities for research trainees and the ability to engage the public on topics of global importance in which chemistry plays a critical role.

Effective management of the center is crucial to generating outcomes that are greater than the sum of what individual investigators might achieve. This aspect is particularly important given the scope of the investment in CCIs. Over the 2013-2015 three-year window, 13.7% of the CHE division budget was expended on centers. The current review process and program management are to be commended for their work in promoting the importance of synergistic interactions. As the first generation of CCIs are reaching their end, it is essential to have a critical assessment of whether they did achieve the desired synergy and what effective strategies might be implemented in the future to enhance the outcomes and benefits of these centers.

Educational mission

Nearly all programs within the NSF have significant educational components. The training of students at all levels, K-12, undergraduate, graduate and post-doctoral, will have a

profound impact. Fundamental and transformative research is the foundation of chemistry. The education of the next generation of scientists is enriched and refreshed by substantive involvement of students and faculty in research.

The Research Experiences for Undergraduates (REU) program in particular can empower a highly diverse population in terms of gender, URMs, and source institutions, to an extent that many other NSF programs cannot accomplish explicitly. The strong focus of the REU program on the experience of the participant, in the context of the science, makes this program particularly inviting and transformative for those who otherwise are significantly disconnected from the scientific research endeavor. For a student in a college where research is virtually nonexistent, the REU program can be the essential first step into real chemistry. A quality REU experience can instill a passion for solving complex scientific problems. The combination of an REU and a continuous research experience is valuable in helping students to make the appropriate choice of a post undergraduate career in research as a graduate student, in industry as a trained employee, or in other pursuits as a citizen better informed of the nature and challenges of science and engineering.

The inclusion of K-12 involvement in the focus of many broader impact activities has the potential to significantly enhance the breadth of the impact of NSF resources, as long as these initiatives include a continuing and well-considered involvement in the community. Support for these outreach programs is essential for the development of relationships and self-identification by the K-12 programs as members of the scientific community.

Overall, the educational impact of the Division's programs is far-reaching. More qualified and skilled participants produce better informed adults who have the potential to discover science as a career and thereby can bring about transformation and innovation for future generations. In addition, high-quality outreach has the important effect of educating the general population on the value of chemistry so that they may make informed decisions in government and business.

Chemistry instrumentation

Almost all chemistry research is dependent on instrumental measurements. Acquisition of modern instrumentation is essential to a vibrant chemical research enterprise conducting high-impact, fundamental research. The primary way the Division supports instrument acquisition is through the Major Research Instrumentation (MRI) program. The MRI program provides separate allocations of funds to support instrument acquisition at PhD granting institutions and PUIs. About half of the awards go to PUIs, which is very important to maintaining their research and education programs.

PIs may be able to obtain smaller equipment through individual research awards; however, the size of these awards and the decrease in most budgets relative to the initial request limits the possibility of instrument acquisition. The Division formerly supported instrument acquisition through a separate Chemical Research Instrumentation and Facilities (CRIF) program. Since discontinuation of this program, the Division has augmented its MRI allocation, thereby allowing it to fund more proposals in the MRI competition. Program Officers who oversee the MRI program actively seek co-funding opportunities within NSF to maximize the number of awards that can be made. Their

efforts to maintain an excellent balance within all aspects of the portfolio in terms of types of instrumentation, awards to new PIs and underrepresented groups, geography, and types of institutions must be commended.

The COV observes that many deserving proposals within the MRI program are not supported because of limited funds. The Division's allocation of additional funds for instrumental acquisition has varied from year-to-year. Current funding levels are insufficient to maintain the instrumentation infrastructure needed in chemistry. The COV is concerned about the long-term consequences should this continue and recommends that the Division procure a robust allotment of funds to augment its MRI allocation. The COV also recommends that the Division work with others within the NSF to advocate for increased allocation of funds for instrumental acquisition, especially as it relates to opportunities to obtain more expensive equipment or suites of equipment that are shared by multiple investigators. The Program Officers within the Division who oversee the MRI program are encouraged to continue their proactive attempts at securing co-funding of awards.

International collaborations

The COV recommends that the Division continue and expand its support of international collaborations. Such collaborations foster the transfer of ideas and technologies and also provide opportunities for students to have international experiences. Basic science is a global enterprise, and participation in international efforts is no longer optional. Resources should not be limited to travel and conference participation, but also need to support real collaborative efforts in partnership with national and international agencies. The COV suggests consideration of a model with components similar to the Erasmus and Horizon 2020 Programs of the European Union to support international cooperation and mobility.

Industrial collaborations

The Division should continue efforts to support partnerships between academia and industry, pursuing and extending the recommendations contained in the 2013 COV report. These efforts will lead to an increase in the level of funding for transformative chemistry through industrial leveraging of the insufficient public funding for this task. Additionally, these efforts will stimulate the demand for highly trained professional chemists and researchers and will extend the focus of graduate programs to further consider industrial opportunities. Whenever possible, the broader impact sections of proposals should identify or include industrial partners.

The COV suggests that mechanisms be employed to stimulate academic and industrial collaborations. Beneficial ways for industrial collaborations to support university research, while reflecting the current state of business, academia, and government policy, should be explored. These efforts should be aimed to reverse the trend of reduced support of basic research by industry.

IV. Response of the Chemistry Division to the 2013 COV Report

Eight recommendations were made by the 2013 COV. Assessment of the Chemistry Division's response to each recommendation is provided below.

Recommendation #1: Find mechanisms to further increase the efficiency and efficacy of the review process. These efforts should include establishing a database of reviewers and developing mechanisms for educating the reviewer pool on the importance of substantive reviews and reviews that provide constructive advice to PIs. An essential aspect of this recommendation is to increase the clarity, transparency and integrity of the review process, particularly with respect to communication to PIs. Two examples are transparency in identification and development of priority research areas and clarification of broader impacts. The Broader Impact criterion is an important component of competitive proposals, but there remains misunderstanding on what it is and how it is used in evaluation. Moreover, evaluation of the broader impact component should be consistent across programs of the Division. Finally, the Chemistry Division should continue its efforts to ensure that the composition of review panels is as diverse as possible, including members with high-levels of research activity and breadth, as well as young PIs.

The COV finds that the Division has responded to this recommendation with a broad range of activities, including implementation of the reviewer database and reviewer educational workshops, especially for early career investigators. The Division has also responded well to the request for "transparency in identification and development of priority research areas and clarification of broader impacts." The COV applauds these efforts, such as the Food Security report, to address this issue. The COV also applauds the Division for their efforts to ensure that "evaluation of the broader impact component [are] consistent across programs of the Division." An Advisory Committee concluded that a deliberately non-prescriptive approach may benefit the community, as it allows for a variety of responses, as well as the highest level of creativity in satisfying this review criterion. Broader impacts are very difficult to quantify and even to anticipate accurately. This review criterion has now been made clearer in the documentation provided to PIs and reviewers. Nevertheless, there is still confusion within the community about the definition, assessment, and weighting of broader impacts, and further clarifications are warranted. In general, greater transparency in the review process should continue to be pursued.

Recommendation #2: Maintain continuity of Program Officers in programs over a period of time.

The Division's response was appropriate, especially given the advantages of rotators with respect to depth of expertise and current activity in the field.

Recommendation #3: Increase the efficiency of operations and the number of Program Officers to improve program management.

Given the constraints, the response was appropriate. The addition of the AAAS fellow is viewed as a positive step forward in this direction.

Recommendation #4: Reevaluate the distinction between the catalysis and synthesis programs

and investigate best ways to categorize the programs in these areas.

The COV applauds the construction of the joint SYN/CAT panel because it provides necessary reviewer and Program Officer expertise.

Recommendation #5: Reevaluate the timing of the submission windows.

The response was appropriate given that the Division is constrained by logistical issues in this regard.

Recommendation #6: Commission a National Academies review/study of the Realignment of the Chemistry Division.

The response was appropriate.

Recommendation #7: Work to increase more industrial partnerships. The division should consider: (a) using Centers even more effectively to bring about university/industry engagement; and (b) examining best practices at NSF to help facilitate faculty/industry partnerships using NSF-facilitated internships.

The representation of industrial collaborations within the Division's center-type grants appears to be sufficient. Requiring individual grants to have industrial connections risks distancing them from the core "basic science" mission, which the committee strongly wants to protect and enhance. Nevertheless, industrial partnerships should be encouraged for the cases when it would be advantageous.

Recommendation #8: Explore ways to increase global engagement of the chemistry community, especially faculty and students involved in projects in other countries.

The approaches used to enhance global engagement have been reasonable, but additional efforts to encourage international collaborations are recommended.

Overall, the response of the Division to the 2013 COV report has been appropriate. In most cases, progress has been made, but further efforts are warranted.

Appendix A: List of Members, Division of Chemistry 2016 Committee of Visitors

Last name	First Name	Institution
Aiken	Karelle	Georgia Southern
Bryant-Friedrich	Amanda C.	U of Toledo
Campbell	Charles	U Washington
Cooks	R. Graham	Purdue
De Bettencourt-Dias	Ana	U Nevada Reno
Eaton	Sandra	U Denver
Ellman	Jonathan	Yale University
Ewbank-Popescu	Codrina	Colgate University
Field	Robert	MIT
Francesconi	Lynn	Hunter College
Haines	David	Wellesley College
Hammes-Schiffer	Sharon	UIUC
Harrop	Todd	U Georgia
Johnston	Murray	U Delaware
Laskin	Julia	PNNL
Liu	Yi	Molecular Foundry, LBL
Liu	Gang-yu	UC Davis
McNally	Mary Ellen	DuPont
Mujica	Vladimiro	Arizona State University
Odom	Teri	Northwestern U.
Osborn	David	Sandia National Laboratories
Petersson	E. James	U Pennsylvania
Reisman	Sarah	CalTech
Sisk	Wade	DOE BES
Swope	William	IBM
Valentine	Ann	Temple U
Wenzel	Thomas	Bates College

Appendix B: Charge to the COV

OFFICE OF THE ASSISTANT DIRECTOR
MATHEMATICAL AND PHYSICAL SCIENCES



4201 WILSON BOULEVARD
ARLINGTON, VIRGINIA 22230

NATIONAL SCIENCE FOUNDATION

Charge to the Chemistry Division (CHE) COV

September 4, 2015

By NSF policy, each program that awards grants and cooperative agreements must be reviewed at three-year intervals by a Committee of Visitors (COV) comprised of 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, and are made available to the public. The COV is charged to address and prepare a report on:

- The quality and effectiveness of the merit review process;
- The selection of reviewers;
- The management of the programs under review;
- The management of the overall portfolio including the balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, etc.

Decisions to award or decline proposals are ultimately based on the informed judgment of NSF staff, based on evaluations by 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 evaluation the overall quality of the Division's decisions on proposals, program management and processes, and results.

The review will assess operations of individual programs in CHE as a whole for three fiscal years: FY 2013, 2014, and 2015. The CHE programs under review include:

- Chemical Catalysis (CAT)
- Chemical Measurement and Imaging (CMI)
- Chemical Theory, Models and Computational Methods (CTMC)
- Chemical Structure, Dynamics, and Mechanisms- A and B (CSDM- A and B)
- Chemistry of Life Processes (CLP)
- Research at Undergraduate Institutions Sites (REU)
- Environmental Chemical Sciences (ECS)
- CHE Instrumentation and Facilities
- Macromolecular, Supramolecular and Nanochemistry (MSN)
- Chemical Synthesis (SYN)
- Centers for Chemical Innovation (CCI)

Appendix C: Breakout Groups

First Program Review (Leaders/Scribes in Red)

Program	CAT	Centers	CLP	CMI	CSDM-A	CSDM-B	CTMC	EDU	ECS	INSTR	MSN	SYN
Room	II-525	II-535	II-545	II-565	II-575	II-575	II-585	II-585	II-565	II-545	II-525	II-535
Scribe	Campbell, Charles	Liu, Gang-Yu	Harrop, Todd	McNally, Mary Ellen	Field, Robert	Osborn, David	Mujica, Vladimiro	Aiken, Karelle	Johnston, Murray	Eaton, Sandra	Liu, Yi	Francesconi, Lynn
	Ellman, Jonathan	Petersson, E. James	Ewbank-Popescu, Codrina	Sisk, Wade	Laskin, Julia	De-Bettencourt-Dias, Ana	Swope, William	Haines, David	Valentine, Ann	Wenzel, Thomas	Odom, Teri	Reisman, Sarah

Second Program Review

Program	CAT	Centers	CLP	CMI	CSDM-A	CSDM-B	CTMC	EDU	ECS	INSTR	MSN	SYN
Room	II-525	II-535	II-545	II-565	II-575	II-575	II-585	II-585	II-565	II-545	II-525	II-535
Scribe	Bryant-Friedrich, Amanda	Laskin, Julia	De-Bettencourt-Dias, Ana	Valentine, Ann	Ellman, Jonathan	Petersson, E. James	Ewbank-Popescu, Codrina	Swope, William	Odom, Teri	Cooks, Graham	Reisman, Sarah	Haines, David
	Aiken, Karelle	Johnston, Murray	Eaton, Sandra	Mujica, Vladimiro	Osborn, David	Liu, Yi	Charles Campbell	Field, Robert	Francesconi, Lynn	Liu, Gang-Yu	McNally, Mary Ellen	Harrop, Todd
		Sisk, Wade									Wenzel, Thomas	

Appendix D: Agenda

2016 Committee of Visitors Division of Chemistry Agenda

Tuesday, May 10, 2016

7 - 9 PM (*optional*) Informal Gathering

Wednesday, May 11, 2016

7:30 AM Continental Breakfast for COV Members – Stafford II-555

8:15 AM Welcome – Stafford II-555
Sharon Hammes-Schiffer, Chair, CHE COV
Angela Wilson, Division Director, CHE
Carol Bessel, Deputy Division Director, CHE

8:30 AM Charge to the Committee of Visitors
Fleming Crim, Assistant Director, Mathematical and Physical Sciences (MPS)

8:45 AM Overview of Division – Angela Wilson

9:00 AM Review of Proposals – First Program Review Assignments (see below)

10:30 - 10:45 AM Break, Stafford II-555

11:45 AM Working lunch available in Stafford II-555

1:30 PM Submit First Program Review Report to Chair and move to Second Program Review Assignments

3:00 PM Break, Stafford II-555

3:15 PM Return to Second Program Review

5:30 PM Submit Second Program Review Report to Chair

6:30 PM Adjourn, Dinner

Thursday, March 12, 2016

7:30 AM Continental Breakfast, Stafford II-555

8:00 AM Discussion with Chair and Consolidation of First and Second Program Reports

10:00 AM Break, Stafford II-555

10:15 AM Return to Drafting Report

11:30 AM Question Period with CHE DD/DDD and Staff

12:00 PM Working lunch

2:00 PM Break, Stafford II-555

2:15 PM Briefing the MPS AD, on findings and recommendations, Stafford II-555

3:15 PM Open Discussion of any Divisional issues not covered previously, Stafford II-555

4:15 PM Adjourn

Friday, June 10, 2016

12:00 - 4:00 PM First and Second CLP Program Groups Finalized Report

Appendix E: COV Report Templates

FY 2016 REPORT TEMPLATE FOR NSF COMMITTEES OF VISITORS (COVs)

The table below was completed by program staff.

Date of COV: May 11-12, 2016
Program/Cluster/Section: All programs in CHE
Division: Chemistry
Directorate: Mathematical and Physical Sciences
<p>Number of actions reviewed: 269 (258 projects, 11 collaboratively linked)</p> <p>Awards: 100 (96 projects)</p> <p>Declinations: 160 (153 projects)</p> <p>Other: 9 (9 projects)</p>
<p>Total number of actions within Program/Cluster/Division during period under review:</p> <p>Awards: 1436 (1366 projects)</p> <p>Declinations: 4038 (3825 projects)</p> <p>Other: 135 (130 projects)</p>
<p>Manner in which reviewed actions were selected: A spreadsheet was created of the 5,474 competitive actions (5,191 distinct actions and 283 non-lead linked collaboratives) ascribed by the NSF database to the Chemistry Division in FY 2013 - FY 2015. 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]).</p> <p>Data retrieved for each proposal included the FY, proposal number, PI, 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.</p> <p>A grid was created for each of the reviewed programs, containing as columns the three 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 or current program staff. Single proposals were also drawn from the top (where available) for major initiatives, for EAGERS, and for</p>

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, only the leads of collaboratively linked proposals were considered.

A separate list of proposals returned without review during the COV period (135 proposals, including 5 non-leads) was generated and randomized as above. Where available, one of these was selected in order from the top of the randomized list for each program.

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 without conflicts with the subset of members assigned to this program were put forward.

This process resulted in selection of 249 proposals total, or roughly 5% of the pool. 11 of these (~4%) 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.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Catalysis (CAT)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>The most important issue is choice of knowledgeable reviewers. (See suggestions below.)</p> <p>Positive aspects of ad hoc reviews: Used absolute ranking scale, although normalization of each reviewer with regard to past average ranking would be useful. Avoided large % errors in statistics of small numbers in ranking small numbers of proposals relative to each other with small number on panel.</p> <p>Ad hoc reviews were numerous, usually more than three, and these were most often very specific for the area of expertise. For the mail review of RUI proposals, a more concerted effort should be made to include reviewers from PUIs.</p> <p>Positive aspects of panel reviews: Thorough discussion across a large set of proposals, should generally provide the most thoughtful and consistent reviews, the best spreading of scores, and the most accurate evaluations of relative proposal merit.</p> <p>There seems to be some inconsistency in ranking of awards based on panel comments as well as reviewer comments. The justification for award decisions should be made clear.</p>	<p>Yes</p>

<p>Data Source: Data Provided</p>	
<p>2. Are both merit review criteria addressed</p> <p>a) In individual reviews?</p> <p>b) In panel summaries?</p> <p>c) In Program Officer review analyses?</p> <p>Comments:</p> <p>More definition to guide the creation of broader impacts should be offered in which one of the criteria would be to make activities achievable on the basis of either impact on society via great science that can improve technologies, or Education/Outreach, or combinations of both.</p> <p>The balance in review of the two merit review criteria varied significantly between funded and declined proposals. The review should be more consistent between these two groups. The PO analysis addresses these criteria well, better in more recent years.</p> <p>Data Source: Jackets</p>	<p>Yes</p> <p>Yes</p>
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>It was surprising how little emphasis was placed on past productivity in overall assessment, yet COV views this as highly important. The emphasis on past productivity is significant in renewals and with more established investigators, however in the case of new PIs this is an area that should be weighted appropriately.</p> <p>Some COV members think that the Division should ask for a quantifiable score on past productivity with regard to integrated impact as evidenced by number and quality of publications, citations, invited talks, and awards that recognize research excellence. It is also believed by some that in the case of renewal proposals, there should be two such rankings of productivity based on: (1) most recent associated NSF funding, and (2) overall track record of PI.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>In some cases, too much emphasis was placed on a comment by a single individual in the panel summaries.</p> <p>In one or two cases, overall evaluation by the panel disagreed with averaging of reviewer ratings. A reviewer's evaluation of a proposal might change after the panel discussion, but the evaluation and score might not have been revised to reflect this. Of course, it might also be expected that the views of the panel are not always aligned with the individual reviews.</p> <p>More consideration should be given to the total number of proposals reviewed per panel. Excess workload for panelist can make the reviews less substantive. However, very low numbers of proposals do not offer a significant basis for comparison.</p> <p>Some of the COV members encourage the POs to consider the statistics of small panels. For example, if 30% of the proposal in the whole program can be funded, then only 3 on average should get funded in panels that treat only 10 proposals. The standard deviation on this number 3 is nearly 2, so this means that anywhere from 1 to 5 out of the 10 in any given panel could be in the true top 30% of the larger proposal set from the whole program. Therefore, choosing the top 3 proposals out of 10 is not completely fair. Doing so would often result in awards to 2 proposals that were not in the true top 30% overall, and other panels where awards are not given to 2 proposals that are in the true top 30% overall. Thus, one needs to treat larger sample sizes if using a 'cutoff' in order-ranked proposals.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>When rankings do not correspond to funding outcomes, PIs should be given, in writing, very clear explanations on how the funding decision is made.</p> <p>For panel discussions, ranking of the proposals in a panel is crucial and was usually provided by the program officer. Some COV members think that explicit rankings should always be provided. For example, in the COV jackets reviewed, unfunded proposals were occasionally "scored" better by individual reviewers</p>	<p>Yes</p>

<p>than some of the funded proposals. Concern was somewhat alleviated by the Review Analysis, which also took into account the panel rankings. Without ranking information, outcomes could appear to be arbitrary.</p> <p>Data Source: Jackets</p>	
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<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>Some COV members think that the PIs should be provided with explicit rankings from panel reviews. Without this information decisions have the potential to appear arbitrary (see Section 5 above). In written communications from the PO, information on position within the panel ranking would be welcomed by most applicants.</p> <p>In cases when the proposal falls in a specific category it is critical that the PO provide comments to explain why this category was possibly chosen from the panel. It is also important to reference specific statements in the panel summary to indicate why this ranking was obtained.</p> <p>Data Source: Jackets</p>	<p>In part</p>
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<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p> <p>It is noted that panel rankings are not always consistent with the funding decision. When proposals have high rankings or scores, it is very important that decisions not to award compared to lower-scored or lower-ranked proposals be strongly justified to avoid the appearance of arbitrary decisions. Additionally, some issues appear to exist in which funding levels were reduced due to</p>	<p>Partially</p>
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overlap between the proposed work with existing funded research in an applicants' laboratory. The level was decreased to what is considered a standard grant. It is not clear why this would be considered a reasonable solution to overlap.

At every step in the process, the ratings and decisions are backed by substantive critiques of the intellectual merit and broader impact of the proposals. A significant amount of attention is given to the intellectual merit and the broader impact the proposed work will have in the field (intellectual broader impact).

With the exception of RUI's, the program and the reviewers varied in how much weight they gave to the training of students (or outreach) in their consideration of the proposals. In some cases, PIs are commended when they are doing a good/exceptional job in these areas but it does not seem to carry much weight in the final decisions.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>Each area of specialization within catalysis, e.g., heterogeneous catalysis, homogeneous catalysis, materials or organic synthesis, can rely on different experimental approaches and techniques and emphasize different aspects of catalysis. For this reason, a proposal reviewed in a specific area should have some reviewers from the same area.</p> <p>For example, the choice of referees who had the requisite expertise was better in homogenous catalysis than in heterogeneous catalysis, and this resulted in somewhat questionable decisions in the latter area.</p> <p>As another example, a young investigator was organic, but the reviewers were all inorganic. The proposal scored poorly despite an apparent strong publication record based on preliminary results. The area match between the reviewers and PI could have been better.</p> <p>Data Source: Jackets</p>	Generally yes
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>Data Source: Jackets</p>	Yes
<p>3. Additional comments on reviewer selection:</p> <p>Most reviewers were from academia. Some were from National Labs. Importantly, many panels had at least one reviewer from a non-PhD granting institution.</p>	

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.

Comments:

Revise ratings to provide more definition.

POs are encouraged to seek guidance from established databases or other sources to select the best referees with specific expertise.

As noted in the 2013 COV report there is overlap in the Chemical Synthesis and Chemical Catalysis programs, causing some level of confusion. Funded Chemical Catalysis proposals are to a very high proportion and with very few exceptions from PIs with inorganic training and from the inorganic community. Funded Chemical Catalysis proposals appropriately directly focused on intimate aspects of catalysis, mechanistic details and catalyst efficiency. Proposals that employ catalysis to provide access to an expanded range of typically more complex products, e.g., towards natural products/pharmaceuticals, should not be transferred by POs from Chemical Synthesis to Chemical Catalysis unless focus is wholly on the design of new catalysts with detailed mechanism studies planned, rather than focus on the products made.

In FY 2015, the CAT program arranged for one program officer to be assigned to both SYN and CAT. This is viewed as a very important means by which to ensure that all proposals get properly assigned and possibly co-funded. This person also educated potential applicants on the differences between the programs.

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

Comments:

To expand on the previous comment, POs are encouraged to seek guidance from established databases or other sources to select the best referees with specific expertise. This is particularly important in emerging fields for which there is limited expertise.

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

Comments:

Emphasis on heterogeneous catalysis appears low relative to homogeneous catalysis yet has played a much larger role in industrial catalysis and is currently a “hot topic” in worldwide research. There should be some attention paid to the balance of priorities within the program as it relates to emerging trends and national needs.

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

Comments:

The program’s response to the previous COV comments and recommendations was good. For proposals focused on catalyst development, there is now a clearer distinction between synthesis and catalysis. The implementation of the joint SYN/CAT panel for cross-disciplinary proposals is applauded and now provides the necessary reviewer and PO expertise.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

Balance across disciplines

Attention is given to interdisciplinary themes as demonstrated through co-funding by other directorates. Funding for heterogeneous catalysis is less than that for homogeneous catalysis, yet it has played a much larger role in industrial catalysis. Some COV members think that there should be more attention paid to the balance of priorities within the program as it relates to national needs.

Projects that integrate research and education

The focus is much more on research than on education, as appropriate for the basic science mission of the NSF.

Award size and duration

Awards to new and early-career investigators

The award sizes seem appropriate. It is commendable that award duration and size is made to fit the programs of each individual investigator, allowing for flexibility in education and research training. It should be mentioned that research funding and duration are tied to productivity as related to publications, which is not to the advantage of early career investigators unless weighted properly for years in research, which is generally done by reviewers. The number of proposals submitted by new investigators as well as the number of awards seems reasonable.

Awards to different types of institutions

Some of the COV members are concerned that in 2014 and 2015, the top 100 PhD institutions accounted for ~70% of awards, and funding of PhD granting institutions that do not belong to the top 100 account for approximately 15% of awards. In some years the numbers of proposals submitted from these latter institutions are also very low. This was not the case in 2013, where the top 100 PhD institutions accounted for only 55% of the awards.

With the BSLFO category, it is difficult to determine the correct distribution of institutions as Research Offices for many institutions fall in this category.

Innovative/potentially transformative projects,

Many of the reviewers cited innovativeness of the projects to justify their recommendations. Based on the documentation (PO Review Analyses, Reviews, Summaries, etc.) projects had to be

potentially transformative or exerting a potential positive impact on the field in order to warrant funding.

Projects with elements of risk,

This is difficult to evaluate. In general, projects that were deemed to have insufficient preliminary data for proof of concept were denied funding. It is not clear whether the projects were necessarily “risky” because in most cases, the reviewers required preliminary data to prove that the idea could work to some extent.

Inter- and multi-disciplinary projects,

*Same as above for “**balance across disciplines and sub-disciplines**”:* ~14% of the awards were co-funded by other directorates. This demonstrates that CAT gives attention to the interdisciplinary nature of the awards where appropriate.

Projects that integrate research and education,

CAT is more focused on research, as appropriate for the mission of the NSF. The education component of the projects was not given as much weight in the award/decline decisions.

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

While reviewers noted that some of the proposals mentioned outreach to women and minorities without clear plans for doing so, this did not appear to be given much weighting in the final decisions.

The reviewers also commended PIs who were broadening participation through their projects. Even though this may not be an important part of the decisions, it is good that the reviewers are taking note of PI’s who are doing a good job of this and letting them know.

Projects that are relevant to agency mission or national priorities

The reviewers looked for innovation and projects that could provide significant breakthroughs in the area of catalysis. Many of the proposals, including those awarded, also targeted sustainability, the creation of more “environmentally-friendly” chemistry, and clean/renewable/alternative energy.

OTHER TOPICS

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.
2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.
3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

A. The 2013 COV report said that the NSF should work to improve transparency and improve confidence in the review process. We agree with this assessment. The following suggestions reflect the opinions of some but not all of the COV members.

(I) Some COV members thought that reviews should be released immediately after the panel meeting and before funding decisions are made. In this way the PI is immediately provided with clear guidance on scientific direction. Also, PIs with either poorly or very highly scored proposals would then have an immediate understanding of the likelihood for funding. This procedural change would greatly improve transparency.

(II) When reviews are released from panels, in addition to reviewer evaluations and ranking (E, V, G, F or P), the much more precise and informative overall percentile ranking should also be released to the PI (this is automatically released to PIs by the NIH). Consistent release of percentile ranking would greatly increase transparency and improve confidence in the review process.

(III) Effectiveness should be weighted most heavily in Education and Outreach; novelty and innovation without effectiveness has no value.

(IV) As noted in the 2013 COV report, the availability of other support to the reviewers is complicated. Reviewers should be advised as to under what circumstances it is or is not appropriate to consider "other support" when evaluating merit and ranking proposals. Funding overlap if identified should of course be noted and relayed to the program officer (see below).

(V) As administered by program officers, there is sometimes inconsistency in allowable research overlap between awarded NSF proposals and the corresponding PIs' other funded and/or submitted proposals (NSF, NIH, DOE, etc).

NSF may ask for some more quantifiable scores on past productivity with regard to integrated impact as evidenced by publications, citations, invited talks, and awards that recognize research excellence. All of these can reflect the intellectual merit and broader impacts of the work. Some reviews contained very little substance.

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.

The format of the data provided by each program was sometimes not meaningful for interpretation of specific trends in demographics and funding. The percentage of women and URMs within their individual groups was presented but not as a percentage of the total number of awards made. It would be important to present this data in both forms for evaluation.

The information for geographical distribution of awards would be enhanced by information concerning the number of grants submitted from each state as well as the number of awards made. This would help to determine if outreach in under-funded areas is needed

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Centers for Chemical Innovation (CCI)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>The COV feels that the number of reviewers and method of review is appropriate at each stage of the CCI award considering the number of proposals and the amount of the award. Each stage of the review process works well for evaluating the strengths and weaknesses of proposals. In phase I, additional cyber review of CCI grants occurs. Phase II proposals are evaluated by more than 15 reviewers (mail and panel). Furthermore, panel members participate in a site visit. A site visit, or reverse site visit, is certainly necessary and appropriate for evaluation of Phase II proposals, considering the amount of support involved. Given the geographically distributed nature of the centers, the reverse site visit is probably the only reasonable mechanism for reviewing these proposals. The opportunity to ask questions of and observe the interactions of the investigators and their students/postdocs is very important to determining whether acceptable levels of collaboration are occurring.</p> <p>Data Source: data provided</p>	Yes
<p>2. Are both merit review criteria addressed</p> <p style="padding-left: 40px;">In individual reviews? Yes, written reviewers specifically provided separate comments regarding intellectual merit and broader impacts.</p>	Yes

<p>In panel summaries?</p> <p>Yes, summaries specifically provided separate comments regarding intellectual merit and broader impacts.</p> <p>In Program Officer review analyses?</p> <p>Yes, both areas were addressed in detail in the review analysis of these proposals. Center grants also require additional review criteria, such as collaborations and grand challenges.</p> <p>Comments:</p> <p>The COV was particularly impressed by the depth, insightfulness and thoroughness of the Review Analysis.</p> <p>The amount of comments provided by reviewers, panels, and program officers (POs) on intellectual merits and broader impacts was appropriate and sufficiently specific.</p> <p>Both merit criteria were addressed in the reviews. However, while the programmatic expectations for the intellectual merit are higher for CCI than for individual proposals, it does not seem to be the case for broader impacts.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>The reviewers of all proposal jackets examined provided justifications for the scores given to proposals, both on intellectual merits and broader impacts. While the extent of comments provided varied by reviewer, it was considered sufficient in all cases, particularly for the intellectual merit.</p> <p>The scoring practice of individual reviewers may vary and is difficult to calibrate and normalize, but most reviews remain consistent.</p> <p>The reviewers provided specific feedback, although in many cases their ability to do so was limited by the relatively low level of detail in the project descriptions as compared to an individual investigator application.</p> <p>Data Source: Jackets</p>	Yes
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p>	Yes

<p>Comments:</p> <p>Panel summaries were sufficient to represent the consensus and substantiate critiques of all individual reviews. The COV considers the panel's judgement to be sound, especially regarding how to rank proposals facing similar overall scores, and how to scientifically judge conflicting views presented by the individual reviews. One area of improvement is to ensure that the final paragraph of the panel summary conveys the relative weights of the critiques.</p> <p>Data Source: Jackets</p>	
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The documentation does a very good job in providing context for the decisions, particularly those "on the borderline." For example, in one case the panel was split, with only some recommending funding. The PO's review documented the issues that divided the panel as well as the additional criteria taken into consideration when making the funding decision.</p> <p>Data Source: Jackets</p>	Yes
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The reverse site visit and the "hot topics" list provided to the PIs two weeks prior to the visit seem to be a very fair way of giving the PIs every chance to address critiques of their application. The hot topics allow the PIs time to prepare their remarks for the panel, but not make substantive changes to their program. Since the PIs have feedback before the reverse site visit, the panel summary and conversations with the PO are the main mechanisms for their understanding of the outcome of the review.</p> <p>Data Source: Jackets</p>	Yes
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p>	

Overall the review process is very thorough, fair, and well-documented. The COV panel agreed that the POs did an outstanding job to ensure that CCI remain true to its areas of focus, i.e., chemistry, innovation, transformative work, and targeting “grand challenges.”

The COV compliments the quality and effectiveness of the CCI review process, especially considering the volume and complexity of CCI proposals. The COV was very impressed by the POs’ analyses of reviews and panel reports. Scientific reflections made by the POs on comments from the reviewers were thorough and insightful. The amount of time spent on these large and interdisciplinary proposals by POs is substantial.

The COV panel is impressed by the decision making judgement of the POs in the case of similar reviews to discern key intellectual merits and broader impacts, in conjunction with innovation, multiple chemistry disciplines, and leadership qualities, to ultimately select highly successful CCI teams.

The POs and panels have emphasized the “center-ness” of proposals (i.e., if the total is greater than the sum of the individual parts). The COV feels that this is entirely appropriate for CCI projects.

Since some CCI applications that are very strong overall may have weak sub-projects, the PO should have discretion in at least encouraging the PI to reassess the allocation of funds to that sub-project.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>The COV notes that finding reviewers for CCI is particularly challenging, given the high likelihood of COIs and higher time-commitment required by reviewers. The CCI POs consistently managed to obtain a large number of high quality reviewers having appropriate expertise. There is an appropriate mix of experts and generalists.</p> <p>Data Source: Jackets</p>	Yes
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>The process is very comprehensive and dynamic. In one case, an unforeseen conflict was discovered during the panel discussion and was appropriately addressed and documented. Another complicated COI case was fully documented in the Jacket with a specific and effective course of action.</p> <p>Data Source: Jackets</p>	Yes
<p>3. Additional comments on reviewer selection:</p> <p>The POs should continue to ensure that the full range of expertise is represented in the review process even if some reviewers are only able to comment on specific parts of the proposal.</p> <p>The COV supports the current practice of inviting all Phase I PIs of CCI projects as reviewers of Phase II applications the year before they are to submit their own Phase II application.</p>	

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.

Comments:

The COV compliments the successful management of the CCI programs by the POs. The COV notes that this is a difficult program to manage, since the number of grants is very small, and the importance of having the impact and synergy make the research center-worthy adds an additional burden. The decision to forego Phase I competition in FY13-15 reflects the harsh budgetary reality. It appears to be a very responsible decision so as not to penalize the previous Phase I recipients vying for Phase II grants. It seems (from review analysis and diaries) that there is good communication between CCI POs and POs in other Chemistry areas which is important to selecting appropriate reviewers and also providing opportunities for declined proposals to pursue applications for individual grants or small collaborations. We commend the hands-on and active role POs play in following up with CCI teams to provide feedback regarding the strengths and weaknesses, as well as advice for improvement. The POs take a much more active role in advising the members of a CCI than is typical for individual grants, which is appropriate. Site visits and attendance of CCI meetings by the POs are necessary and important to monitor progress and provide timely feedback and advice for the CCI teams.

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

Comments:

The CCI program provides a much needed mechanism to encourage and support research to take on grand challenges and to solve complex scientific problems in chemistry, where other funding mechanisms are rarely available.

Obviously, the hiatus for Phase I applications severely hindered the program's ability to respond to emerging opportunities, so it is heartening to hear that Phase I applications may soon be accepted again. For education, the program should provide channels for different CCIs to work together to capitalize on valuable outreach strategies. The program is encouraged to continue exploring opportunities for leveraging resources.

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

Comments:

The portfolio is diverse and dependent on the quality of proposals submitted in response to the CCI call.

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

Comments:

Overall the 2013 COV was very positive about the CCI program. They recommended increased staffing and continuity of POs for this large and long term program. The increase in staffing does not seem to be in the budget, but PO continuity seems good (and management of some CCIs by other POs helps to distribute effort and build in expertise in case of a change in primary PO). They also recommended increasing inclusion. While the PIs tend to be at large research institutions, many investigators on CCIs are at smaller schools and those that serve underrepresented populations. This has improved with the larger number of Phase II CCIs now funded and may have been more effectively presented to the 2016 COV by looking at the total distribution of investigators.

Only one point in the NSF's response to the 2013 COV report explicitly mentioned CCIs, a call for more synergistic collaborations with industry. This seems to have been strongly considered for many CCIs, especially those with industrial representation on advisory boards. This issue has been satisfactorily addressed in the October 2015 response letter that highlighted some of the results of the CCI-industry collaborations.

The previous COV recommended strategic planning because of the small number of awards and their high profile. As new calls for Phase I proposals emerge, an analysis of the CCI portfolio will be essential to ensure that Phase I funding is directed to new challenges. Co-funding with other agencies may be possible (e.g., with BIO for brain-directed projects). This would help to address a recommendation of 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."

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: *balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities*).

Questions about portfolio are difficult to address for a program with such a small number of grants. The portfolio is diverse with a strong focus on transformative science. The COV is pleased to see 5 minority-serving institutions and 5 primarily undergraduate institutions participating in CCI among 57 currently funded institutions. It is also noteworthy that among 166 faculty members funded by CCI, 40 are female and 14 are underrepresented minorities. The COV encourages the program to continue broadening the range of investigators and topic areas funded by CCI.

OTHER TOPICS

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

Due to the small number of projects, there are necessarily gaps in this program. The COV encourages the POs to broaden the range of topics funded by the program through the upcoming call for Phase I proposals. Projects combining experiment and the development of new theories are underrepresented in the current portfolio. The POs are encouraged to help identify possible interactions between different CCIs in sharing best practices and resources, for example, in support of outreach activities and broader participation.

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

The CCI program places a premium on the value of synergy, namely that the total of a CCI's productivity should be greater than the sum of its parts. This is not an easily measured objective. However, a way of measuring synergistic interactions within CCIs should be established, and the results should be communicated to the community.

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

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

In many cases, CCIs may create unique infrastructure that is difficult to reproduce elsewhere due to cost and expertise. Finding ways to leverage this by making it accessible to the broader scientific community would increase the value of NSF's investment.

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

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemistry of Life Processes (CLP)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>All proposals are reviewed a minimum of three times by a combination of panel and ad hoc mail reviews. Looking at the data, the review process appears to be primarily through panel reviews (2.73 reviews/proposal) with secondary mail reviews (0.88 mail reviews/proposal), which averages to 3.61 reviews/proposal. This number is appropriate.</p> <p>Additionally, 572/761 (75.2%) proposals received panel summaries. Thus, a majority of submitted proposals were discussed at panel. The mail reviews were properly requested, although the number of late reviews and declined reviews was sometimes large. From the data provided by NSF for 2013-2015, we made the following observations about mail reviews:</p> <p>(i) 44% of requested mail reviews get returned;</p> <p>(ii) 22% were returned late in 2014. However, in 2015, the fraction of reviews that were late was much lower than in 2014.</p> <p>(iii) The mail reviewer is not present during panel discussion. However, this critique is muted by the secondary level review/analysis performed by the POs.</p> <p>Additionally, for EAGER and INSPIRE mechanisms, the reviews were waived, and POs reviewed and made the decision. Seeing only one of each of these proposals is not sufficient to make a judgment about the criteria for the decision. Seeking an ad hoc review from an expert reviewer to aid the PO in the funding/decline decision will be helpful and should not delay the decision process.</p>	<p>Yes</p>

<p>Data Source: Data Provided</p>	
<p>2. Are both merit review criteria addressed</p> <p>In individual reviews? In most reviews both criteria are addressed; however, in some reviews the broader impacts are either not addressed or very broadly evaluated (see below). For instance, in some cases, where there are enough concerns about the intellectual merits in the mail reviews, the broader impacts are less analyzed in the reviews.</p> <p>In panel summaries? Yes. In panel reviews both criteria are considered.</p> <p>In Program Officer review analyses? Yes</p> <p>Comments:</p> <p>Both merit review criteria are addressed. In several reviews, the critique of the broader impacts is significantly less detailed than that addressing the intellectual merit criterion.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>These reviews are complete for the most part. There were a few instances, however, where the proposal was highly ranked (MRR > 4.5), but was declined based on lack of preliminary results and/or a poor broader impacts section. Additionally, there are some reviews that are summarizing aspects of the proposal and do not give critical evaluation. Finally, most of the substantive comments address the intellectual merit and provide less detail on the broader impacts.</p> <p>Data Source: Jackets</p>	<p>Yes (for the most part)</p>
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Yes. The panel summaries provide the rationale for the consensus of the panel discussions.</p>	<p>Yes</p>

<p>Comments:</p> <p>Face-to-face panels are different from virtual panels in many ways:</p> <ol style="list-style-type: none"> (1) Social dynamics in virtual panels may work differently than in face-to-face discussions. Discussion may be more difficult; people who are younger or quieter by nature may speak less, which influences the quality of the discussion. This is the experience of some members of the COV team, while others had different experiences. (2) The length of the discussions of individual proposals in virtual panels may depend on the program officer and director. It is very important that the virtual panels consider and allocate time for the relative ranking analysis after the discussions of individual proposals, similar to what is done on site. (3) From the panel summaries that were seen by the COV, it appears that they provide a rationale for the consensus. The writing of the Panel Summary at the end of the virtual panels relies heavily on the Program Directors to marshal the panelist to write comments for the scribe. This is the experience of some members of the COV team, while others had different experiences. <p>The experience with any panel seems to be directly correlated with how it is run by the POs.</p> <p>Data Source: Jackets</p>	
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>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.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The Review Analysis is generally very good, although it does not reach the PI.</p> <p>It is recommended that the PO use the Review Analysis to provide more substantial comments to the declined PIs to allow the latter to better understand the reason for the decision and eventually to resubmit a more competitive proposal at a future time.</p> <p>Data Source: Jackets</p>	<p>YES</p>
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p> <p>Given the E, V, G, F etc. ratings and based on the reviews we have seen, we recommend that NSF provide clear direction to reviewers:</p> <ul style="list-style-type: none"> (1) to spread their ratings and (2) to provide comments consistent with the ratings or alternatively adjust the ratings to reflect panel discussions. <p>In panels, the PO has the important role of ensuring that all panel participants are heard.</p> <p>Overall, the multi-step process of reviewing is sound and followed with care.</p>	

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>The COV team commends the program officers and directors for handling the complicated reviewing process in an efficient manner. The discussion of the proposals shows that the reviewer expertise was sufficient and that the panel mechanism provides opportunity for sharing expertise.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>Within the proposal, there is a special section called “List of Suggested Reviewers and Reviewers Not to Include”. This section is often under-utilized. It would be helpful if the GPG could make clear that putting reviewer names in this section does not influence negatively the review process. This will especially assist early-career applicants.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>3. Additional comments on reviewer selection:</p> <p>Selection of reviewers is not an issue of representation, but one of education. In proposals submitted from PUIs or schools with an MS program, there did not appear to be enough representation of PIs from these types of schools on the panel. However, the number of proposals from PUIs in each panel is too small to have more PUI reviewers. Overall, there was a concern for balance in selection of the reviewers, particularly for RUI and CAREER. 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 bias we have about what type of student and what type of institution can produce good chemical research and train the future great scientists.</p> <p>The statistics for funding for FY13-FY15 provided by the POs (pre-COV) are: 2 year schools 33% funding rate (only 3 proposals submitted) 4 year schools 18% funding rate MS schools 7% funding rate PhD schools 20% funding rate (PhD-granting schools among the top 100 recipients of NSF support in a given year have 30% funding rate.)</p> <p>The lack of disparity between 4 year and PhD granting institutions seems to indicate that panel reviews are not problematic for PUIs, although there is no indication of how many of the PUIs are private institutions; the low funding rate for MS granting institutions is a reason for concern, as it might indicate a lack of knowledge of their circumstances by the reviewers. Proposals from the top 100 schools fare significantly better than those from other schools.</p> <p>There is no information about balance in the reviewer pool from the point of view of race, gender, type of institution (private vs. public, research versus PUI), competence in the field, and geographic.</p> <p>The response rate and quality of reviews vary over a broad range. We suggest that the Division could use the internal database of reviewers to store the history of recommendations (E, V, G, etc.) of each reviewer. In addition, in this database, the POs may use an internal grading system, by which the POs assess the quality of the reviewers.</p>	
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III. Questions concerning the management of the program under review. Please comment on the following:

MANAGEMENT OF THE PROGRAM UNDER REVIEW
<p>1. Management of the program.</p> <p>Comments:</p> <p>Management is appropriate. The POs are doing an excellent job of managing the review process and organizing face-to-face and virtual panels.</p>
<p>2. Responsiveness of the program to emerging research and education opportunities.</p> <p>Comments:</p> <p>The responsiveness is also appropriate.</p> <p>It seems that the community, in the form of the reviewers, guides the responsiveness.</p>
<p>3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.</p> <p>Comments:</p> <p>The selection is largely defined by the quality of the proposals. The PO judgment is particularly important for proposals that are at the border between being recommended for funding or not.</p>
<p>4. Responsiveness of program to previous COV comments and recommendations.</p> <p>Comments:</p> <p>The COV found that the NSF is working on the previous COV recommendations. In particular, one problem raised again by us concerns Broader Impacts. The recurrence of this recommendation suggests that it is difficult to address and that further effort is needed.</p>

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 714 proposals over the last three years, of which 168 were awarded for a funding rate of 23.5%. This number is in-line with the Division of Chemistry funding rate, which is 26.2% (1436 awards/5474 submitted). These awards are appropriate in terms of total dollars (\$148,600/year) and duration (3.2 years). These numbers are slightly below the total dollar amount (\$162,800/year), but in-line with duration (3.1 years) for Division averages. CLP includes a sizeable number of awards that are funded through other directorates (BIO (main) and ENG, MPS-CHE-CDS&E, MPS-CHE-CSDM-A, MPS-CHE-CAT, among others) for a total funds-out of \$5,659.40 (K per year) and funds-in of \$8,559.70 (K per year).

The portfolio does have a reasonable national award distribution with funded states on the West Coast (CA, OR, WA), Southwest (TX), Midwest (WI, IN, OH, MI), Southeast (GA, NC) and Northeast (NY, MA, PA, MD). However, there is a neglected section of the country to which no CLP-funded grants have been awarded (and perhaps from which no applications have been received), especially in the Plains States (ND, SD, NE), parts of the West (ID, NV, NM), Southeast (MO, AR), and AK and HI. It is recommended that the program targets these states better.

Of the awards made, the majority has gone to Research Intensive (Top 100) PhD institutions (121/168 awards = 72.0%) with 4 year schools (6/168 = 3.6%), and Masters Institutions (5/168 = 3.0%) rounding out the top three. In general, these numbers reflect the percentage of submitted proposals by these types of institutions: Research Intensive (Top 100) PhD, 367/714 = 49.3%; 4 year, 33/714 = 4.6%; Masters, 70/714 = 9.8%. More effort should be made to increase the number of submitted and funded proposals to these non-PhD institutions.

New investigators are slightly underrepresented, which is demonstrated by the 18.3-18.4% fund rate of CLP proposals that are in the new or new involvement PI category, compared to the overall CLP rate of 23.5%, and considering that 365/714 = 51.1% of submitted proposals are from new or new involvement PIs.

The funding rate of women (23.0%) and underrepresented minorities (20.3%) receiving CLP awards is mostly in-line with the CLP overall funding rate of 23.5%, the Division funding rate for women and minorities (26.2 and 21.4%, respectively), and the overall Division funding rate of 26.2%. Naturally, these numbers must be improved to reflect the increasing number of women and minorities entering STEM disciplines.

OTHER TOPICS

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.
2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.
3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.
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.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Measurement and Imaging (CMI)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>In some cases, a comparison of results for different panels seems off-centered. Perhaps this is just the nature of the system, but some very high ratings coupled with strong statements in the reviews on some panels did not equate to the award being given, whereas on other panels, seemingly low ratings and less enthusiastic comments were awarded.</p> <p>In addition, panel summaries resulting from deliberations provide more discussion of strengths and weaknesses.</p> <p>There was a marked unevenness in how the program was run across the years. In 2013 and 2015, there were panels run (2.45 and 2.02 panel reviews per proposal, 0.76 and 0.64 panel summaries per proposal) similar to the average for CHE. In 2014, mostly mail reviews were used (0.51 panel reviews per proposal, 0.13 panel summaries per proposal). The committee was concerned about fairness and consistency in the face of such fluctuations.</p> <p>Data Source: information provided by program</p>	<p>In some cases.</p>
<p>2. Are both merit review criteria addressed?</p> <p>In individual reviews?</p>	<p>Yes</p>

<p>In panel summaries?</p> <p>In Program Officer review analyses?</p> <p>Comments:</p> <p>a) In individual reviews, yes, comments are provided explicitly for the three fields, intellectual merit, broader impacts and summary statements.</p> <p>b) In panel summaries, yes.</p> <p>c) In Program Officer review analyses, yes both review criteria are explicitly addressed by the program director.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>Yes, for intellectual merit. However, it appears that some proposals/jackets fared better when the reviewers were more brief in their overall remarks. In other proposals/jackets, reviewer remarks were not treated in an equivalent manner.</p> <p>For some proposals, if a comment was made about something that could be addressed, it was considered not pertinent. For others, it was considered substantive enough to decline the proposal.</p> <p>Data Source: Jackets</p>	Not always
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus:</p> <p>Comments:</p> <p>Panel summaries explicitly list strengths/weaknesses for intellectual merit and broader impact and a rationale for the panel summaries. Since the majority of the proposals were reviewed by virtual panels, it would be helpful to clarify the duties of a virtual panel when the panel convenes, i.e., real-time interactive. Design of the virtual panels may be specific to NSF, but may not be consistent with other organizations.</p> <p>Data Source: Jackets</p>	Yes

<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The documentation does provide the rationale for the award/decline decisions. Some rationales were not consistent with panel reviews or recommendations. In those cases, the review analysis suggested separate criteria that are not consistent with NSF's goals, although program balance might have been the factor.</p> <p>Such rationale might be used for a supplemental equipment proposal but is not ideal for an initial proposal award.</p> <p>Data Source: Jackets</p>	<p>Most of the time.</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The documentation to the PI in the form of the panel summary and the individual reviews is adequate.</p> <p>No site visits were noted in proposal declines or awards.</p> <p>Data Source: Jackets</p>	<p>Yes.</p>
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p> <p>Reviewers and program officers are working very diligently to get a fair and precise review of the proposals submitted. But what is considered excellent by one panel may equate to good or even fair by another. There needs to be more guidance on what a review evaluation means by defining the relative terms of excellent, very good, good, fair and poor and what they mean. The assignment of E/VG or VG/G suggests that reviewers are searching for a more precise means of delineation. Although this might be unrealistic, trying to normalize the opinions of the reviewers would be a good idea. Worthy individuals may</p>	

disagree about the best way to achieve this goal. Clearly the Program Officer's judgment and expertise are crucial.

The review analysis of some proposals included a description of the CMI program "Review Process" (i.e., the 9 virtual panels, total number of proposals submitted to CMI). However, this was not necessarily included in other review analyses. Its inclusion seems to depend on the Program Officer writing the analysis. Standardization of what information should be included in the review analysis should be considered, along with uniform written dissemination of pertinent information to PIs.

When awards receive joint funding, it would also be helpful if the review analysis described the relationship with another program, e.g., ICC, 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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>In general, the reviewers appeared to be very knowledgeable about the material that was being reviewed.</p> <p>The Program Officer sometimes carried out ad hoc reviews rather than panel reviews for unusual proposals. This may have led to the large changes in the way that proposals were reviewed, specifically the proportion that were reviewed by panels vs. by mail reviews from year to year.</p> <p>Data Source: Jackets</p>	Yes
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>No unrecognized or unresolved conflicts of interest were identified.</p> <p>Data Source: Jackets</p>	Yes
<p>3. Additional comments on reviewer selection:</p>	

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

MANAGEMENT OF THE PROGRAM UNDER REVIEW
<p>1. Management of the program.</p> <p>Comments:</p> <p>It would be helpful to understand the process of when proposals are sent for ad hoc reviews and when they are chosen for panel review. Within the ejacket system, if ad hoc reviews are solicited and never returned, they should be removed from the review category of pending to cancelled after a reasonable period of time.</p>
<p>2. Responsiveness of the program to emerging research and education opportunities.</p> <p>Comments:</p> <p>Some proposals' awards were definitely skewed towards more experienced PIs. CAREER awards in the CMI programs definitely address emerging research; some effort should be made within NSF to identify and support mid-career level scientists.</p>
<p>3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.</p> <p>Comments:</p> <p>Where priorities were articulated (funding a less-funded new investigator versus funding an already-well-funded investigator), they seemed to be reasonable. To a large degree, the POs have little control over what is submitted because most proposals are unsolicited.</p>
<p>4. Responsiveness of program to previous COV comments and recommendations.</p> <p>Comments:</p> <p>The 2013 COV recommended to CMI that reviewers be encouraged to offer constructive (as opposed to dismissive) criticism. The current COV did not note any reviews that were other than constructive.</p>

The report also recommended establishing a reviewer/panelist database that is easy for POs to work with. That has not been done fully for various reasons outlined in the responses, and would still be a valuable goal.

The 2013 COV raised a concern about the lack of continuity with respect to the Program Officers in CMI. There have again been changes over the three years evaluated by the current COV, but no adverse effects to the program were noted.

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

Please comment on portfolio balance considering balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities.

The awards are appropriate in duration but are funded at a size (\$149K/yr) that is lower than average for CHE (\$162.8K/yr). The portfolio includes a number of inter- and multi-disciplinary projects, as is reasonable for its scope and mission. Cooperation with two other directorates and eleven other chemistry programs are noted. The geographic distribution, awards by type of institution, balance of awards to new investigators, and participation by underrepresented groups are all in line with norms for the CHE division.

OTHER TOPICS

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

The program needs to consider the evaluation of GOALI, RUI versus each other as opposed to general review in panel or ad hoc from collaborative or individual proposals.

Industrial research dollars are diminishing inside organizations, but support from Industry for a GOALI suggests there is an end-use need and should be weighted heavily in a review.

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

No additional comments.

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

Consideration should be given to getting rid of the Excellent, Very Good, Good, Fair and Poor categories and considering using a strictly whole number system 1 through 5. The categories are calculated to a numerical system in the Review Analysis typically, and this would be clearer to the reviewers and to the PIs.

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

Perhaps a better vetting of websites and passwords to simplify the process would be helpful prior to sharing with COV panel members.

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

With regard to balance across disciplines and sub-disciplines in the CMI program, it would be helpful to know the distribution of current awards across the 8 areas (represented by 9 panels) as well as funding success rates for each area. It would also be helpful to know which areas suffer from underrepresentation such that remediation measures, i.e., educating the community, could be implemented. One area of concern is the dearth of instrument development proposals and awards, although this is an area of support in the CMI programs description: "Topics also considered by CMI include the development of new instrumentation enabling chemical measurements likely to be of wide interest and utility to the chemistry research community." Of the roughly 620 proposals, approximately 16 of them were self-identified instrument development proposals, and 3 were awarded.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Structure, Dynamics and Mechanisms A (CSDM-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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>We believe that the best possible review procedure incorporates a mixture of mail reviews and panel. The panel provides a basis for questioning and possibly lowering the weighting of a review that is clearly biased or incorrect. This is extremely important because proposers are unable to respond to an unbalanced or incorrect review. It gives the Program Officer authority to disregard a defective review.</p> <p>Panel: One negative aspect of panels is that one or two panel members can have an inappropriately large influence on the discussion in the panel. In addition, mail in reviews are often not given appropriate weight in the panel discussions. We are concerned that there are often only 2 mail in reviews.</p> <p>Ad-Hoc: One negative aspect of ad-hoc reviews is that each ad-hoc reviewer evaluates only a few proposals without the ability to discuss with fellow reviewers, and thus it is not possible to evaluate relative merit across a program, spread scores, or reach a consensus on key issues such as the purpose or impact of the rather ill-defined Broader Impacts criterion.</p> <p>Data Source: data provided</p>	

<p>2. Are both merit review criteria addressed</p> <p style="padding-left: 40px;">In individual reviews?</p> <p style="padding-left: 40px;">In panel summaries?</p> <p style="padding-left: 40px;">In Program Officer review analyses?</p> <p>Comments:</p> <p>We found that both intellectual merit and broader impacts criteria are addressed. However, we believe that no one really understands what “broader impacts” means. This is especially problematic because reviewers and panelists often use their own concept of “broader impacts” to downgrade a proposal.</p> <p>Especially in mail-in reviews, the weighting broader impacts has on the final score could vary dramatically, whereas in a panel review the PO can guide / enforce a more uniform assessment of broader impacts. We feel there is room for improvement in the transparency of how broader impacts are evaluated.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>Most reviews are substantive. However, several very brief, non-reasoned, extreme positive or negative reviews are submitted. The Program Officer should have the authority or even the requirement to disregard such reviews and to put into the file a comment about the reliability of that reviewer. We have noted that the review analyses by the Program Officer often provide criticism of worthless reviews, but it is unclear whether the Program Officer has the authority to not include the rating of such a proposal in the computed average rating.</p> <p>Data Source: Jackets</p>	

<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>The panel summaries were mostly accurate and insightful. When the sense of the panel in the ranking of the proposal deviates from the final funding decision, the panel summary should and usually does provide a clear justification.</p> <p>Data Source: Jackets</p>	
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The documentation in the jacket is a clear and useful record of the basis for the Program Officer's decision. In a very small number of cases, the funding decision seemed at odds with the information in the jacket, possibly owing to unspecified programmatic balance issues.</p> <p>There is one issue of including RUI proposals in a panel of mostly R-1 proposals. There is a genuine risk that R-1 criteria are inappropriately applied to RUI proposals, and that this seems to not be addressed anywhere in the material in the Jacket. Separate panels, or some other administrative arrangement, for RUI and R-1 proposals should be considered.</p> <p>We echo sentiments of other members of the COV that the reviewers of an RUI-only group of proposals should still be diverse (i.e., not only RUI-reviewers), and include some reviewers from R-1 and other research intensive institutions.</p> <p>One CAREER proposal was first reviewed by ad hoc reviewers and received high scores but was declined. A revised proposal was then submitted and reviewed by a panel, received mediocre scores, and was funded. Careful reading of the review analysis shows reasonable rationale for this decision.</p> <p>This proposal is a clear example of why the COV recommends that the Review Analysis information, redacted only as much as necessary, be communicated to the PI. Otherwise the decisions of the Program Officer may appear to the PI to be somewhat arbitrary, when in fact they are made with considerable thought.</p> <p>Data Source: Jackets</p>	

<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The comments from the Program Officer to the PI of declined proposals are usually minimal. However, such documentation could be extremely valuable, and more attention to this is warranted.</p> <p>We recommend that as much as possible of the Review Analysis be given to the PI. We understand that telephone conversations are always offered to those PIs who have been declined. We furthermore understand that such conversations rarely take place, and hence are of little value in helping declined PIs improve their next proposal. Therefore, we recommend being as transparent as possible by providing as much of the Review Analysis in writing to the PI as possible.</p> <p>The comments to the PI are not always completely consistent with the PO review analysis. For example, in one case a PI received mostly positive scores but was declined. The review analysis presented both scientific criticisms and grant overlap as reasons for declination, but grant overlap was not relayed in the written PO comments.</p> <p>Data Source: Jackets</p>	
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p> <p>Overall we were impressed with the quality and accuracy of the merit review process. However, non-substantive and fallacious reviews continue to be a pernicious problem.</p>	

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>We are concerned with the difficulty of obtaining a sufficient number of high quality, uniquely qualified reviewers. Some new mechanisms should be explored to increase the number of such reviewers. One COV member suggested requiring (at risk of some penalty in the consideration of future proposals) a specified number of substantive reviews from every PI of a successful NSF proposal within 5 years of the start date of that grant.</p> <p>In two cases we noticed that a proposal from a less well-known institution was reviewed by reviewers from other similarly ranked institutions (including one reviewer in an engineering department), whereas the very well-known PIs from highly ranked institutions generally have well-known reviewers from similarly ranked institutions. Some of this difference may be due to the difficulty of finding expert reviewers for less-known PIs from less-known institutions. But an effort should be made to ensure that reviewers and PIs are not “stratified.” For other cases, the reviewers and the PIs were NOT stratified, so this problem is not pervasive.</p> <p>Data Source: Jackets</p>	
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>It is not clear from the jackets how conflicts of interest were addressed.</p> <p>Data Source: Jackets</p>	
<p>3. Additional comments on reviewer selection:</p>	

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

MANAGEMENT OF THE PROGRAM UNDER REVIEW
<p>1. Management of the program.</p> <p>Comments:</p> <p>Mostly we are impressed with the way in which the program is managed. However, there have been a small number of cases where bias about the vitality of research area played a role. There were a few cases where the decision process was not transparent. However, often the review analysis provided sufficient information, but it was not relayed to the PI in the PO comments.</p>
<p>2. Responsiveness of the program to emerging research and education opportunities.</p> <p>Comments:</p> <p>Yes! We are impressed by the number of proposals co-funded by different programs at other NSF agencies. The program funds research at the frontiers of knowledge. It is important to be aware of the relatively long time constant for emergent areas to become appreciated by the reviewer community.</p>
<p>3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.</p> <p>Comments:</p> <p>There appear to be insufficient funding resources to solicit proposals in specific areas. This places severe limits on the efforts of Program Officers to encourage new initiatives.</p>
<p>4. Responsiveness of program to previous COV comments and recommendations.</p> <p>Comments:</p> <p>There are detailed responses to the previous COV recommendations, but most of the recommendations were stated to be outside of the administrative and fiscal capabilities for response from this NSF program.</p>

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

OTHER TOPICS

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas. No comment.
2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.
3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

One COV member proposed that reviews should be released immediately after the panel meeting and before funding decisions are made to facilitate the PI's scientific planning. In this way the PI is immediately provided with clear guidance on scientific direction of the proposed research. Also, PIs with either poorly or very highly scored proposals would then have an immediate indication of the likelihood for funding. This procedural change would greatly improve transparency.

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.

More (succinct) guidance would have been appreciated. Some COV members did not realize that the past COV reports and responses, as well as the filled-out templates from the past reports, were provided via links sent to the COV members prior to the meeting.

Navigating the eJackets was extremely time consuming. It would be helpful if a single (reduced) pdf for each program could have been prepared for each COV panelist that includes reviews, review analysis, and panel summaries of each proposal. The COV recognizes that creating such a single PDF for each program could be administratively time consuming if done manually, but the PDF generation could potentially be automated with a clever script.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Structure, Dynamics and Mechanisms B (CSDM-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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>The review of CSDM-B proposals changed from essentially all mail-in for 2013 to almost entirely panel-based (with some additional mail-in reviews) in 2014 and 2015. The COV believes that a combination of in-person panel reviews for all (or nearly all) proposals, supplemented with at least one mail review by an expert in the field of the proposal, is the best way to ensure both a fair relative ordering of the proposals and ensure topical expertise among reviewers. For expediency during review panels, we like the practice of triaging proposals into high, medium, low, and do not discuss further categories. This should save the panel time to focus more on the competitive proposals. However, there should always be the opportunity for panel members to reconsider any submitted proposal. One COV member suggests that the Program Officers should consider a policy that if any panel reviewer believes a proposal initially placed in the "do not discuss further" category should be reviewed, this proposal receives at least two reviews.</p> <p>Data Source: data provided</p>	Yes
<p>2. Are both merit review criteria addressed</p> <p style="padding-left: 40px;">In individual reviews?</p> <p style="padding-left: 40px;">In panel summaries?</p>	Yes, usually

<p>In Program Officer review analyses?</p> <p>Comments:</p> <p>In most cases, the reviews address both criteria. However, the individual reviews do not always separate intellectual merit from broader impacts. In many cases, very different weight is given to the two categories (usually much more focus on intellectual merits than broader impacts). While the PO can only exercise so much control over the individual reviews, we saw great variability in the panel summaries as well. In this case, the PO must make sure that the panel conversation takes appropriate consideration of both aspects. It is also important for the PO to make sure that the intellectual merits and broader impacts are clearly defined for the panel.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>In general, the reviewers' comments were found to be substantive and often helpful. In several cases, PIs were given ideas for how to improve a future version of a proposal not recommended for funding. We note that the NSF does not have control over this aspect beyond requesting that reviewers provide substantive comments.</p> <p>Data Source: Jackets</p>	Yes, usually
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>The COV finds the quality of the panel summaries to be variable. In many cases, the panel summaries are quite descriptive and summarize the main strengths and weaknesses, along with some suggestions for improvements in the case of both approved and declined proposals. In other cases, panel summaries are very short, mostly describing what the proposal contained rather than explaining the reasoning for the panel's recommendation. It is important that the POs encourage consistency and instruct the scribe to make clear which points were important in influencing the panel's overall recommendation. When new suggestions for specific improvements arise during discussion, it is valuable for the panel summary to include this feedback since it will not be in the individual reviews.</p> <p>Data Source: Jackets</p>	Yes

<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The COV finds that the documentation in the jacket (particularly the Review Analysis) provides a reasonable rationale for the award/decline decision. Given the importance of the Review Analysis in understanding this rationale, we suggest that more information be provided to the PI (see below).</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The COV finds that the individual reviews and panel summary can be valuable feedback for the PI, but we would like to encourage the Division to provide additional information to the PI regarding the PO's analysis. The Review Analysis is typically an insightful summary of the strengths and weaknesses of the proposal, summarized from the key points of all the reviews. As COV members, we found these Review Analyses very helpful, and we were surprised to see that this information is NOT provided to the PI. The PO Comments are probably meant to convey this information to the PI, but they tend to be much shorter and less detailed than the Review Analysis. While certain parts of the Review Analysis may need to be redacted, we feel that the concise summary the PO officer has written could be very helpful to the PI in revising or creating future proposals. This is especially important if the individual reviews were lacking in detail and/or there is no panel summary. In the end, the PO makes the decision for or against funding, with the reviews being his/her advisory opinions. The insight into the key reasoning behind the PO's decision is crucial feedback to the PI. The Review Analysis contains this information, and we think it would be helpful to the PI to see as much of this information as possible. It may also be valuable for the PI to be told the relative ranking of his/her proposal (even in very general terms).</p> <p>Data Source: Jackets</p>	<p>Not always</p>

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

In general, the COV found the review process to be thoughtful and credible. In particular, we found the Review Analysis showed a substantial depth of thought by the PO. The COV commends the implementation of a more panel-based review process. We are particularly impressed with what appears to be a more efficient review process since there has been a reduction in the number of POs with an increase in submissions. We see that good management by the PO can be essential to providing a fair review process and clear feedback to the PI. Keeping the panel aware of review criteria is very important to this management. In general, we see that the POs have done an excellent job of this in recent years.

Again, we emphasize the value of transparency from the POs in communicating information beyond what is found in the reviews to the PIs. Occasionally, there is an outlier negative review among other reviews that are quite positive. In one case, the PO comments did a good job of explaining why the negative review did not have a significant influence on the decision. In another, the F review was mentioned, but only a very brief explanation was given as to why it was discounted. It is important to consistently provide context so that the PI can understand the rationale for the funding decision and take appropriate action to improve his/her proposal effectively.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>In general, the reviewers seem to have appropriate expertise. The use of some mail-in reviewers is important in a program such as CSDM-B where unusual (or even unique) technical expertise can be essential to reviewing the intellectual merits of the proposal. However, we feel that it is beneficial to balance this with a panel review that can debate the proposal’s merit relative to competing proposals and impact on the field in general. A spectrum of panel members at different stages of their careers and at different types of institutions can provide this balance.</p> <p>Data Source: Jackets</p>	YES
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>We found no problems with the conflict of interest requirements.</p> <p>Data Source: Jackets</p>	YES
<p>3. Additional comments on reviewer selection:</p> <p>As the community becomes more collaborative, there are increasing problems with conflict of interest, which creates problems in finding appropriate reviewers/panelists and even POs for all proposals.</p>	

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

MANAGEMENT OF THE PROGRAM UNDER REVIEW
<p>1. Management of the program.</p> <p>Comments:</p> <p>It is worth noting that the number of POs decreased from 4 to 3 (from 2014 to 2015) and the number of proposals increased from 115 to 131. This is a 53% increase in proposals/PO/year. The review of the 2015 proposals appeared to be of high quality, so this may reflect increased efficiency. However, it does raise concerns about the POs being overburdened.</p>
<p>2. Responsiveness of the program to emerging research and education opportunities.</p> <p>Comments:</p> <p>There are two relevant issues here. One is publication of calls for proposals that encourage applications that focus on emerging areas that the Division values. The other is in changing priorities for the fields of individual reviewers. Informing researchers of new funding priorities and informing reviewers of NSF-wide strategic plans can help to make the proposal submission and review process responsive to emerging opportunities.</p>
<p>3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.</p> <p>Comments:</p> <p>We did not see a clear vision statement that would allow us to address this.</p>
<p>4. Responsiveness of program to previous COV comments and recommendations.</p> <p>Comments:</p> <p>The report from the 2013 COV is very thorough, and the recommendations issued seem to have been addressed in part or in full in the response letter. We did not see any CSDM-B specific concerns that were not met. The significant change in moving to the use of panels seems to have been implemented well.</p>

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

The CSDM-B program has a well-balanced portfolio, with a few aspects noted as below:

Review methods: The program review switched from primarily mail-in review in 2013 to panel/mail-in review in 2014. This is a positive and recommended move.

Award size: Both award number and size goes up every year. There might be local variations in between individual awarded proposals, but it does represent a good and healthy trend. The award size (~131K) is however smaller than the average in CHE (~163K).

Inter-disciplinary projects: CSDM-B has a much larger amount of incoming funds than outgoing funds. These projects may require more than usual staff time to manage, but the POs managed it well.

Geographical distribution: The CSDM-B has a relatively small number of awards, thus even distribution across different regions is not possible. Midwest regions do show lower statistics in terms of numbers of awards. No data on geographical distribution of submission was available to compare the acceptance rate by regions.

Type of Institution: Awards were fairly well balanced across different types of institutions. There were significantly lower numbers of submissions from institutions other than PhD institutions.

New PI and early-career PIs: New PIs have a slightly lower acceptance percentage than the average, and the number fluctuates by year. This could be tracked back to inexperience in proposal writing, or lack of preliminary results, and seems to be a common theme (also observed in other programs such as MSN). The COV commends efforts by Program Officers to provide useful advice to all proposal writers, but especially to novices.

The average CAREER award rate in CDSM-B for FY13 – 15 was 22.8%. This value is essentially identical to the overall success rate of 23.4%.

OTHER TOPICS

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.
2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.

We noticed that one EAGER proposal was reviewed only by a knowledgeable Program Officer, but not by a panel or external reviewer. This proposal was declined without further review. Some COV members feel that an EAGER proposal that meets all pro-forma requirements should receive at least one outside or panel review.

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

A recent article in the news detailed how some NSF programs went to a no-deadline format, which decreased the number of applications and thus increased the funding success rates. Some COV members wondered if this approach could be evaluated for broader usage throughout the NSF.

Lengthening the duration of awards (e.g., to 4-5 years) could alleviate some of the burden on reviewers, PIs, and POs.

There continues to be uncertainty among both PIs and reviewers as to the relative weight of broader impacts versus intellectual merits as evaluation criteria.

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

One perspective from the COV was that there is a trend to require broader impacts that are more specific to applications. Some fraction of fundamental research can be easily linked to applications, but there are significant areas that are, at the moment, purely curiosity-driven research with no clear application. The NSF must make an effort to value these impacts that may have less of a "pop-science" spin.

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

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Theory, Models, and Computational Methods (CTMC)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>In comparing individual vs panel reviews, some of us tend to favor the latter because it reduces the risk of bias, while others prefer ad hoc reviews because those reduce the risk of decisions based on a dominant personality.</p> <p>A panel that treats 10 proposals (selected from a larger population that should have 30% funding rate) will have anywhere between 1-5 out of the 10 that are actually within the top 30% of the larger population, simply due to the statistics of small numbers. (The standard deviation of 3 is almost 2.) Therefore, the decision to fund amongst a group of 10 by rank order (e.g., funding the top 3 out of the ten) is subject to huge errors, due to the statistics of small numbers. With such a small set (ten), one needs some absolute score that has more statistical significance.</p> <p>Some COV members think that it would be more significant if reviewers' scores were normalized based on each reviewer's historical average. A recommendation would be to renormalize the individual scoring systems of each reviewer, because the same proposal could be rated either "excellent" or "good" depending on the makeup of the panel, thereby affecting the funding odds for the proposals.</p> <p>Some COV members also think that one way to make the ad hoc reviews have an attractive aspect of the panel reviews (without actually having a panel) would be to send all of the reviews to the reviewers and ask for a second review that addresses the other reviewers' comments.</p> <p>Data Source: data provided</p>	<p>Yes</p>

<p>2. Are both merit review criteria addressed</p> <p>In individual reviews? Yes. In panel summaries? There were proposals (in the Declined category) for which the Panel Summary was absent. In these cases it was not clear whether the proposal was discussed in the panel and rated as DNR, or simply was not discussed in the panel (ND).</p> <p>Second, some panels in this program seem to have a very laconic style in the summary of the panel discussions, compared to panels examined in another program.</p> <p>In Program Officer review analyses? POs compensate whenever the Broader Impacts are not well addressed.</p> <p>Comments:</p> <p>We suggest that the Broader Impacts criterion be achievable on the basis of either Impacts on society via great science and its potential to impact technology or Education / Outreach, or combinations of both. When there is international collaboration, reviewers have a harder time deciding whether that is a broader impact.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>As a general comment, reviews are of variable quality and substance, compared to another program.</p> <p>Reviewers' comments that are communicated to PIs need to be both more specific, constructive, and actionable. Too general comments in the review are especially harmful for new PIs and young researchers.</p> <p>It was surprising how little emphasis was placed on past productivity in overall assessment, yet the COV views this as highly important. It would be useful if the NSF asked for some quantifiable score on past productivity (relative to the stage in the PI's career and the type of institution) with respect to integrated impact as evidenced by number and quality of publications, citations, invited talks, and awards that recognize research excellence. For renewal proposals, two separate such scores should be assessed: one specific to the most recent prior NSF grant's productivity, and one based on the PI's overall productivity.</p> <p>Data Source: Jackets</p>	<p>YES, in part</p>

<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>There were proposals (in the Declined category) for which the Panel Summary was absent. In these cases it was not clear whether the proposal was discussed in the panel and rated as DNR, or simply was not discussed in the panel (ND). Second, some panels in this program seem to have a very laconic style in the summary of the panel discussions, compared to panels examined in another program.</p> <p>Data Source: Jackets</p>	<p>Yes, sometimes</p>
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The rationale presented for declination does not always include the consideration of the competition between proposals.</p> <p>Data Source: Jackets</p>	<p>YES</p>

<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>There seems to be a gap between how the decision is presented to the top tier of proposals that are going to be funded and the second tier, which contains the most promising rejected proposals. (In particular, where the panel summary was absent, the PI got little information about technical deficiencies.) We suggest that the documentation to the PIs should have some more detailed guidance on how to improve. This helps developing the next generation of researchers.</p> <p>Data Source: Jackets</p>	<p>See comments</p>
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p>	

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>The selection of knowledgeable reviewers is the most essential step in the review process. One way to identify experts in specific area of a proposal is for the Program Director/Officers to use the Web of Science to search articles in the topic area and sort these by number of citations. This allows one to identify expertise in the subfield amongst the corresponding authors of multiple highly cited articles in that topical area.</p> <p>CMTC has a difficult job in keeping a balance between supporting proposals dealing with theory, models and computational methods. In particular, a “purely” theoretical proposal, without including an explicit application or a computational implementation may have a smaller chance of being funded. This might reflect a somehow generalized perception that computational chemistry and theoretical chemistry are the same.</p> <p>Data Source: Jackets</p>	Yes, in part
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>Data Source: Jackets</p>	Yes
<p>3. Additional comments on reviewer selection:</p>	

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.

Comments:

In general, this is a well-conceived and managed program.

The ratings (E, V, G, F, P) could be improved, because this is an arbitrary scale (i.e., each reviewer has his or her own scale).

One of us has had excellent success in evaluating proposals with the following system, which seems better defined:

5 = "I would argue in favor of funding this proposal"

4 = "I am in favor of funding"

3 = "I could be convinced to fund this proposal"

2 = "I am against funding"

1 = "I would argue against funding"

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

Comments:

The program is responsive enough to emerging fields and education opportunities. A suggestion would be to expand information about solicitation in emerging fields through web sites and workshops, similar to what other government agencies do.

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

Comments:

The program is well conceived in terms of its scientific focus, but has some challenges especially in the geographical distribution of applications to the program, the distribution of applications from different types of institutions, and in the breadth of participation of under-represented minorities and women. The development of the portfolio is limited by the pool of applications. Thus the program solicitations should highlight the importance of the program for the future of chemistry and science in general, so that institutions in all geographical areas have the confidence to hire and develop faculty and students in theoretical chemistry and chemical modeling.

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

Comments:

The responsiveness to previous COV seems to be adequate. One comment though regarding: Rec. # 7 (COV-2013/Oct-2015): Work to include more industrial partnerships. Apparently little has been done in this very important direction, judging by the limited list of examples provided.

Rec. # 8 (COV-2013/Oct-2015): Explore ways to increase global engagement of the chemistry community Far from moving in this direction NSF seems to have restricted its co-funded international collaboration programs. Probably a lot more should be done in the spirit of what the European Union has in place, and also involving regions in which the US has special interest such as Latin America.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

The CMTC program has some challenges, especially in the geographical distribution of applications to the program, the distribution of applications from different types of institutions, and in the breadth of participation of under-represented minorities and women. The development of the portfolio is limited by the pool of applications. Thus the program solicitations should highlight the importance of the program for the future of chemistry and science in general, so that institutions in all geographical areas and of various types have the confidence to hire and develop faculty and students in theoretical chemistry and chemical modeling.

OTHER TOPICS

1. Please comment on any program areas in need of improvement or gaps (if any) within program areas.
2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.
3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

See above suggestions about revising the ranking system.

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.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Environmental Chemical Sciences (ECS)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>This interdisciplinary program used a mixture of virtual panel and mail reviews (with no in-person panel reviews). In-person panels are considered by some to be preferable to virtual panels in that they give better reviews necessary for a diverse program. The number of reviews secured (both panel and mail reviews) was in line with division averages.</p> <p>A notably high number of panel summaries were provided to the PIs (0.79 per proposal, but as high as 0.96 in the most recent year, so that almost every proposal received a panel summary) as compared to the CHE average (0.72 per proposal).</p> <p>Data Source: data provided</p>	Yes
<p>2. Are both merit review criteria addressed</p> <p style="padding-left: 40px;">In individual reviews?</p> <p style="padding-left: 40px;">In panel summaries?</p> <p style="padding-left: 40px;">In Program Officer review analyses?</p>	Yes

<p>Comments:</p> <p>The PO review analyses and panel summaries always explicitly included both, but individual reviews sometimes were not substantive with regard to both criteria. Some panels did not delineate strengths and weaknesses clearly.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>In general, the reviewer base seemed uneven. There were too many reviews of proposals (declined and awarded) that were either too short or not substantive. The exception was in the case of the CAREER proposals, where the reviewers and reviews provided excellent feedback for declined and awarded proposals.</p> <p>There were several proposal situations of concern, where the reviewers rated the proposal as excellent but did not comment further. Then, the panel concurred with the high rankings but did not provide other comments. However, the proposals were declined. The PO did an excellent job justifying this negative decision, but such instances can cast doubt on the review process.</p> <p>In addition, there were situations where the reviews were weak compared to the award decision by the PO, and the PO did not adequately justify the positive decision.</p> <p>It was not clear in one case why a review was not released.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>Overall, the panel evaluations were often not substantive and simply repeated (verbatim) content from the ad hoc reviews. The panel evaluations were usually too short with little content to aid the PI for future submissions or the PO for funding decisions.</p> <p>However, proposals that were generally favorably reviewed but not funded often had the most useful panel reviews and summaries.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>The COV appreciated that there were direct quotes from the panel and ad hoc reviews in the summaries because it shows what the PO valued and what influenced the decision. The PO read the reviews carefully. Overall, the PO prepared a thoughtful analysis of the intellectual merit and broader impacts for both declined and awarded proposals.</p> <p>The review analysis sometimes contained rationale based on other proposals/ grants by the PIs that was not addressed in the panel or ad hoc reviews.</p> <p>There were, however, many instances in both awarded and declined proposals of a mismatch in ad hoc/panel review and PO decision. In the cases of the proposals that reviewed very well but were declined, the COV agreed with the PO decision; however, the reviewers should have been selected differently to avoid such scenarios. In the cases of the proposals that reviewed weakly or had reviews with little content but were awarded (in full or in part), the COV feels that better justification was needed.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>Yes, although these comments were usually very brief and could benefit from some additional information contained in the review analysis.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>7. Additional comments on the quality and effectiveness of the program's use of merit review process:</p> <p>Better guidance about budget comments from the ad hoc reviewers would be welcome. Some reviewers make those comments. How are those used? Should there be a separate section on the form so that when reviewers are compelled to make those comments, they don't have to put them into the Intellectual merit? It is not clear whether such comments are welcomed or not.</p>	

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>It seems that some proposals were funded in collaboration with other entities within NSF. However, it wasn't clear whether or not such cases were jointly reviewed and therefore needed reviewer expertise from the perspective of the various NSF programs involved.</p> <p>While we recognize the interdisciplinary nature of this field, proposals to a chemistry program should be reviewed by a significant number of chemists. Occasionally, the reviewers tilted toward other areas of science.</p> <p>Data Source: Jackets</p>	<p>Yes; See comments</p>
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>No unrecognized or unresolved COIs were identified.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>3. Additional comments on reviewer selection:</p> <p>Reviewer quality was often poor, where either the review was not commensurate with the rating (just a summary of the proposal and given an E) or there was very little content</p>	

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.

Comments:

It is not easily clear what is a materials proposal versus an environmental proposal. Some clarification would be helpful. For example, does an environmental proposal include significant study of exposure of the material to an environmental system? Some proposals seem to be materials development proposals that may have an environmental application. The materials-type proposals did not fare well; does that mean they should be reviewed elsewhere? The program and the panels should perhaps focus on ECS proposals.

It may be that proposals are accepted into this program but really should be redirected elsewhere. Partly this is a poor choice on the part of the submitting PI, but either the proposal doesn't fare well at ECS or it does get funded and draws resources that should go to true ECS-focused proposals.

It is evident that Fiscal Year 2014 was an outlier in terms of awards made. The percentage of proposals funded was very uneven from year to year. It is recognized that in a small program with limited program officer support, there should be a better backup plan to keep the program running smoothly when unexpected situations arise.

Most importantly, the individual investigators working in an area should not be adversely impacted by a lack of support by the program officer, or lack of support to the program officer and the program from CHE and from NSF overall.

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

Comments:

Emerging research is largely defined by the ECS community and by the proposals that are submitted. High quality proposals were funded. A wide range of proposal types (RUI, GOALI, CAREER) was supported at some level.

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

Comments:

We note that the three-year average percentage funding rate for proposals in this program was lower than the CHE average (23% for ECS vs. 26.2% for CHE overall), and also the average annual dollars per grant is lower than the CHE average (\$130.1K for ECS, \$162.8K for CHE overall). These values, taken together, suggest that this program is under-supported.

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

Comments:

There was much discussion in the previous report about going to panels, and it seems panels are more fully embraced now. This program uses exclusively virtual panels as opposed to in-person panels.

Documentation to the PI was an issue raised by both the 2013 and 2010 COV and may have improved but could still always be further improved. How to explain balance? How to best help the PIs? In general, the documentation does say how the proposal can be strengthened.

The community continues to be confused about Broader Impacts, how to handle them, and how to evaluate them.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

(Questions are taken from the PowerPoint presentation provided by ECS)

1. Does the program portfolio have an appropriate balance of awards across disciplines and sub-disciplines of the activity?

Fiscal Year 2014 stands out for its low funding percentage (10%). The low funding rate was partially compensated with a high funding percentage in 2015 (32%) but such fluctuations are not good for the ECS community.

2. Are awards appropriate in size and duration for the scope of the projects?

The awards are of comparable duration to the CHE average but are significantly lower in size (\$130.1K per year versus \$162.8K for the CHE average). More resources should be directed to this program.

4. Does the program portfolio include inter- and multi-disciplinary proposals?

There is cooperation with one other directorate (GEO) and two other programs within CHE.

5. Does the program portfolio have an appropriate geographical distribution of Principal Investigators?

The geographical distribution seems appropriate given the small number of proposals in ECS.

6. Does the program portfolio have an appropriate balance of awards to different types of institutions?

The program portfolio has a distribution of different types of institutions that is comparable to the distribution in CHE overall.

7a. Does the program portfolio have an appropriate balance of awards to new investigators? (New PIs only)

New investigators did better than average as new PIs in 2013 and 2015, and much less well in 2014, with an overall average close to the CHE average.

7b. Does the program portfolio have an appropriate balance of awards to new investigators? (PIs and co-PIs)

New investigators did better than average as PIs and co-PIs in 2013 and 2015, and much less well in 2014, with an overall average close to the CHE average.

9a. Does the program portfolio have an appropriate participation of underrepresented groups?

The ECS has a participation of women and underrepresented minorities that is similar to that of CHE overall. Further increased participation should be encouraged in all CHE programs.

OTHER TOPICS

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

Nothing noted.

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

Nothing noted.

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

This program is demonstrably underfunded, as shown by both the percentage of proposals that are supported and by the level of support offered to the proposals that are supported. The previous COV stressed the importance of ECS, and we would like to reinforce this importance.

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

Nothing noted.

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

Nothing noted.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Educational Activities (EDU)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>REU: Panel reviews were far richer than the mail reviews. The volume of proposals reviewed by the panel as a whole and individual reviewers were appropriate. There were 8-9 proposals per reviewer and 18-21 proposals per panel. The panels consisted of 9-10 members. The "Review in Context" sections in 2014 and 2015 that were specific to the REU was very informative, and the POs should continue to include this information in their analyses.</p> <p>OTHER EDUCATION: This was mail reviewed. There were inconsistencies in what the reviewers were looking for. While adequate, the review of this proposal would have been enhanced if the reviewers had come together, even by teleconferencing. The suggestion is that such a large project should be panel reviewed.</p> <p>CHEMISTRY PROJECTS: This is a great example of where a panel discussion was extremely valuable in the decision to fund. There were mail reviews followed by a panel review which provided a rich discussion of conflicting opinions. When decisions were made not to discuss a proposal in the panel, the individual reviewers expressed a significant consensus.</p> <p>Data Source: Data Provided</p>	<p>Yes</p>

<p>2. Are both merit review criteria addressed in individual reviews?</p> <p>Comments:</p> <p>REU: There needs to be a stronger emphasis on the review of scientific content. There are different ways to accomplish this. We suggest that the PO strongly encourage the reviewers to evaluate the scientific merit of the proposals, and return the reviews if this condition is not met. Reviewers should at the very least summarize and evaluate the scientific content. Otherwise, for the most part, both criteria were addressed. There were some reviews that were very lacking. There are inconsistencies in what individual reviewers consider broader impact versus intellectual merit. However, they all comment on each criteria.</p> <p>CHEMISTRY PROJECTS: Both the intellectual merit and broader impacts were addressed in the mail reviews and the proposal that was individually reviewed. The reviewers were consistent in what they considered intellectual merit versus broader impact in terms of the innovativeness of the science.</p> <p>OTHER EDUCATION: The reviewers clearly addressed the strengths and the weaknesses of both criteria.</p> <p>In panel summaries?</p> <p>REU: These were consistently done well. However, as stated above, there needs to be a stronger emphasis on the evaluation of the scientific content.</p> <p>CHEMISTRY PROJECTS: When the proposal was discussed in the panel, the summary addressed both the intellectual merit and broader impacts. They commented on the quality of the science and the potential contribution that the proposed work could have on efforts to create more sustainable chemistry.</p> <p>OTHER EDUCATION: No panel summary. Only Mail reviews.</p> <p>In Program Officer review analyses?</p> <p>REU: The Program Officer comments on the strengths and weaknesses of the proposal in the analyses. While not clearly identified, elements of both the intellectual merit and broader impacts are used to validate the PO's recommendation.</p> <p>It is especially important that the PO explains the decision to decline proposals that received high ratings, "E," and the PO does a good job of this.</p> <p>CHEMISTRY PROJECTS: The Program Officer clearly addresses the intellectual merit as well as the broader impact. The PO condensed the comments of the mail reviews and panel summary. In some cases, the PO referred to the reviewers' comments as justification but did not go into detail regarding the intellectual merit and broader impact.</p> <p>OTHER EDUCATION: Absolutely. This is done well.</p> <p>Comments:</p> <p>Data Source: Jackets</p>	<p>Yes</p>
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<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>REU: Most of the reviews were lacking in the evaluation of the scientific content and focused instead on administration and numerics (e.g., number of papers to be written by participants). While these other areas are also important to the success of an REU site, the reviewers should be encouraged to give more weight to the merit of the science in their assessments. A majority of the reviewers provided substantive feedback for the PI's but there were some that were lacking in detail. Some reviewers were brief and did not provide useful input.</p> <p>CHEMISTRY PROJECTS: In all cases, the mail and individual reviews provided substantial feedback that clearly addressed strengths and weaknesses of the proposal under both merit review criteria. Reviews that addressed each criterion for a specific call separately were better in this regard. There were only a few reviews that were not informative.</p> <p>OTHER EDUCATION: All reviewers for this proposal gave substantive information regarding strengths, weaknesses and specific actions that could be undertaken to improve the idea. However, the focus of each review was very different and here again, a panel review would have given more cohesive feedback.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>REU: Panel summaries were very appropriate and provided a good sense of the priorities of the panel and in what ways the proposal did or did not fulfill those priorities.</p> <p>CHEMISTRY PROJECTS: <i>Same as above.</i> The panel did a good job of indicating where panelists were in agreement and disagreement with the mail reviews.</p> <p>OTHER EDUCATION: Not discussed in a panel.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>REU: The Review Analysis was particularly useful. While the individual reviews provided context, they were not always descriptive of the basis for the final decision. One aspect that is clearly important, but for good reason not reflected in the reviewer comments, is the negotiation of funding options.</p> <p>CHEMISTRY PROJECTS: The Review Analysis provides a clear rationale for award/decline.</p> <p>OTHER EDUCATION: The documentation provided by the reviewers as well as the PO's Review Analysis was quite detailed and very clear.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>For all cases, we want to emphasize that it is very important for the PO to convey specific and constructive feedback to PIs, especially for rejected proposals. We felt that many of the reviews were lacking in substance, and the PO should be responsible for distilling this kind of substance from the reviews and presenting it to the PI.</p> <p>REU: The documentation received by the PI provided important feedback for the decision. The most valuable feedback was provided by individual reviews and panel summaries. The PO's comments were mostly a summary of the individual reviewer's comments and with substantive reviews, this was adequate.</p> <p>CHEMISTRY PROJECTS: The mail and individual reviews, as well as the panel summaries, adequately provided the rationale.</p> <p>OTHER EDUCATION: The comments of the reviewers were clear and detailed, but the foci of the reviews were quite dispersed.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

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

REU: There appeared to be some confusion on the part of both PIs and reviewers on the use of NSF chosen foci in designing REU programs. Some proposals tried to use a single theme and were criticized for doing so inadequately, while others were criticized for creating an artificial connection that was not useful for the goals of the NSF program. Is it really necessary for the research projects to fall under one theme? This question should be clarified for the reviewers and PIs.

CHEMISTRY PROJECTS: This was done well. All of the reviewers were in agreement with what they interpreted as intellectual merit and broader impact in terms of the innovativeness of the science. When there was a call for an international collaboration, it is good that the proposal was critiqued by reviewers with the necessary expertise from the various countries.

OTHER EDUCATION: The reviews were detailed. They indicated the strengths and weaknesses of the proposals and provided generous suggestions for how the idea could be improved. All were very informative reviews but dispersed in foci. A follow-up panel review would have brought all of the ideas together.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>REU: There were some comments by individual reviewers that indicated a lack of understanding of the process of undergraduate research. More attention also needs to be given to the scientific merit of the research projects in the review process. However, for the most part, the expertise seemed appropriate. The majority of the reviewers were from academic institutions. The panels also included people from industry and what seem to be STEM institutes, though to a much lesser extent.</p> <p>CHEMISTRY PROJECTS: The expertise was appropriate, and clearly a lot work was put into getting the right people.</p> <p>OTHER EDUCATION: The review could have benefited from having more reviewers with a background in education. The program included people from educational institutes and academia at various levels, for example people in administration and people from colleges of education. This was a broad spectrum of reviewers, and the breadth was appropriate for a proposal that was seeking to make a strong impact on many levels.</p> <p>Data Source: Jackets</p>	Not always
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>COI issues appear to be handled well.</p> <p>REU: The “Context” statement indicated that conflicts of interest where noted were dealt with in an appropriate manner. When there were conflicts, reviewers did not view proposals, and they left the meetings during the discussions where there were conflicts.</p> <p>CHEMISTRY PROJECTS: Yes. The PO’s Review Analysis noted that panelists</p>	Yes

<p>who had a conflict of interest were asked to remove themselves from the virtual panel when that particular proposal was discussed.</p> <p>OTHER EDUCATION: None indicated.</p> <p>Data Source: Jackets</p>	
<p>3. Additional comments on reviewer selection:</p> <p>For remote panels, with perhaps less chance for conversation, the reviewer selection becomes very important. For panels in which discussions can occur on a range of issues, a greater variation of understandings can be accommodated. It is important to have panels whenever possible to bring all of the different ideas together.</p>	

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.

Comments:

REU: The program officers seem well informed and were able to communicate decisions and priorities well. The program aims to fund 20-25 sites per year and has remained close to this goal with an average of 20 proposals per year during 2013-2015. It is notable that the POs have also secured co-funding from other programs, where appropriate, to assist with achieving this target.

CHEMISTRY PROJECTS: The process seems much more involved in making the decision compared to other programs. NSF has created a support system that accommodates the complexities of the program.

OTHER EDUCATION: A panel discussion would have produced a document that was more useful for the PI.

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

Comments:

REU: Project themes in many of the proposals, particularly those awarded funding, target relevant and emerging fields/concerns in science and the broader society.

The point of the REU and related programs is to attract young scientists into various STEM fields. One way to do this might be to emphasize global sustainability. We see that students are excited about environmental issues, and these programs provide a good way to tempt them into a scientific career.

A particular goal of the REU is to broaden participation in STEM. It is clear in the review process the panelists seek to ensure that this is being done at the proposed sites under review. This is performed well.

CHEMISTRY PROJECTS: These proposals clearly address issues of sustainability and were quite appropriate for this call.

OTHER EDUCATION: In some reviews, there was discussion of "Best Practices," as if these were set in stone and agreed upon by all. There is no context for knowing what is meant by the use of this term, but it seemed to be weighted heavily in a program whose goal should be to develop new Best Practices, rather than entrench old Best Practices. Each reviewer needed to state exactly what s/he meant by best practices.

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

Comments:

REU: There is a concern that the pressure to apply NSF foci to the design of REU programs is restrictive.

The women and under-represented minority focus was clear and was consistently and strongly applied.

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

Comments:

Recommendation #1: Find mechanisms to further increase the efficiency and efficacy of the review process.

REU: The Context Statement provided to the PI helps to address this recommendation. In addition, providing the individual reviews is particularly helpful in assisting the PI with understanding how a particular project was evaluated.

Apart from specific scientific projects that all reviewers critique under intellectual merit, there are inconsistencies in what is considered intellectual merit versus broader impact in the reviews.

However, this may not be a significant problem for the REU.

The POs also provided training for the panelists before each review meeting which addresses (i) the difference between broader impact and intellectual merit and (ii) other goals and guidelines for the NSF and the REU in particular.

CHEMISTRY PROJECT: The Context Statement provided to the PIs helps to address this recommendation. There was consistency in what the mail reviewers considered to be intellectual merit and broader impact.

OTHER EDUCATION: The Context Statement provided to the PI helps to address this recommendation. There were inconsistencies in what the mail reviewers considered important.

Recommendation #2: Maintain continuity of Program Officers in programs over a period of time & Recommendation #3: Increase the efficiency of operations and the number of Program Officers to improve program management.

REU: Both recommendations have been addressed. One of the POs has been involved with the program for more than three years and a second PO joined in 2015.

CHEMISTRY PROJECTS: There were at least three POs for each year, and each year had at least one PO with previous experience.

Recommendation #7: Work to increase more industrial partnerships.

REU: The program has included reviewers from industry and institutes. In terms of REU sites achieving this goal, there is no basis to comment on this.

Recommendation #8: Explore ways to increase global engagement of the chemistry community, especially faculty and students involved in projects in other countries.

REU: The CHE-REU program has a number of international sites.

CHEMISTRY PROJECT: This was definitely achieved when there was a call for international collaborations.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

Balance across disciplines and sub-disciplines

REU: The research in various proposals covered all sub-disciplines of chemistry.

Award size and duration

REU: The award duration is the same for all projects, 3 years. Over 2013 to 2015, the program has been able to maintain an average of ~\$90K per award while ensuring that the program remains close to the 20-25 awards per year target. Increasing funding in this area may assist in increasing the number of new REU sites.

CHEMISTRY PROJECT: The awarded proposals were within the scope of the typical award for this program.

Awards to new and early-career investigators

REU: Approximately 35% of proposals submitted during 2013-2015 were from new PIs or/and Co-PI's. Approximately 30% of awarded proposals were led by new PIs/Co-PIs.

Geographical distribution of awards

REU: Awards during the 2013-2015 period are concentrated in the Midwestern, Southern and Eastern regions of the US. It is not possible to determine why this is the case. A broader distribution of REU sites across the country would benefit our young scientists in training. Commendably, the REU program has eight fully international sites.

Awards to different types of institutions

REU: The funding rate for 2-yr. and 4-yr institutions was disproportionately lower than the percentage of submissions.

Few PUI REUs have been funded. Relatively few are applying, perhaps because of the increasing pressure to take few or none of their own students. For PUIs, having an REU program with a cohort consisting of visiting students and students from the home institution will serve to enhance the research experience and output for both groups. The motivation for a graduate school is different. Graduate schools utilize REUs as a recruitment tool, so students from other institutions are often the sole target.

The funding rate for PhD institutions was proportional to the percentage of submissions across all three years. Additionally, there was significant improvement with respect to Master's and top 100 PhD programs. In contrast to 2013 and 2014, the 2015 funding rate was proportional to the numbers of submissions.

Innovative/potentially transformative projects, projects with elements of risk

REU: The greatest risk with REU programs lies in the investment in people. While the program seeks to broaden participation in STEM, it not clear how the CHE-REU as a whole has been able to do this. How many of the students have remained in the field, sought higher degrees, etc.? Based on their comments, the panelists in the review process, however, seem to keep the sites accountable for achieving the individual program goals as well as broadening participation.

CHEMISTRY PROJECT: The reviewers held the PIs accountable for the innovativeness of their ideas.

OTHER EDUCATION: This project was high risk, high reward. This is commendable.

Inter- and multi-disciplinary projects

REU: The CHE-REU has co-funding with other divisions and directorates. This demonstrates that the POs recognize and acknowledge the interdisciplinary nature of many of the projects.

Projects that integrate research and education

REU: All awards during the 2013-2015 period integrated research and education in accordance with the goals of the REU program.

CHEMISTRY PROJECTS:

The project gave attention to the training of students at the high school and graduate level, as well as post-docs. The proposals also gave a good amount of attention to integrating educational activities throughout the year.

OTHER EDUCATION: There was a strong educational component aimed at impacting students at a very early stage in their academic careers across the nation.

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

REU: The participation of women and URM as PIs/Co-PIs has remained consistent with 8-11 and 3-5 awards each year, respectively. Additionally, the sites are reviewed very carefully for their efficacy in broadening participation through the selection and progression of their student-scholars in STEM.

Projects that are relevant to agency mission or national priorities

REU: Overall, the awards during this period show a strong commitment to broadening participation in STEM and engaging undergraduates in rigorous research internships. Clearly the review process holds programs accountable for the quality of research, professional development and recruitment.

CHEMISTRY PROJECTS: The sustainability focus is definitely a national/global priority.

OTHER EDUCATION: This was highly relevant to the agency's goal to train the next generation of scientists.

OTHER TOPICS

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

REU:

On average, the timeline between “received” and “status-date” was between 6-12 months, 6 months in most cases. However, this window was closer to 12 months in 2015. The program officers are encouraged, as much as possible, to provide decisions within 6 months.

High school teacher training: create shorter term assignment possibilities (e.g., two weeks) in order to give high school teachers an opportunity to see real research and instrumentation in action. This will allow them a chance to incorporate new concepts into their lesson plans. Having short two week assignments will reduce the burden of requiring mature high school teachers to be away from home or to travel for an extended period. Perhaps this is something that can be supported with the RET supplement.

A broader distribution of REU sites across the US can enhance the efficacy of the program. It may be that a special emphasis needs to be placed in soliciting proposals from states that did not have awards in the 2013-2015 period.

We want to note that these programs can provide a real benefit to scientists at institutions where research is not the major focus. By supporting even a small amount of research this resource can help to prevent faculty burn out. Perhaps the program could re-evaluate the stipulations on hosting students from the home institution for PUIs. Of course, these school should be held accountable for ensuring that visiting students and those from the home institution are treated equally and that both groups are provided with exceptionally good experiences in the REU programs.

In the selection of reviewers, the program seems to strike a good balance between primarily undergraduate and research academic environments, an average of 30% PUIs over the three years. The POs for the REU are encouraged to keep this balance on each panel. It is likely that both types of institutions can benefit from insight provided by the other in the review process.

Increased tribal colleges' representation in the review process is encouraged. Impressively, there was representation from at least one Minority Serving institution on each panel. These were mostly Historically Black College and Universities (HBCU) and Hispanic Serving Institutions (HSI). The REU is encouraged to continue doing this, ensuring that representation from institutions or programs that serve populations traditionally underrepresented (Native American, Latina/o-American, African-American, Women and Students with Disabilities) in STEM are involved in the review process.

2. Please provide comments as appropriate on the program's performance in meeting program-specific goals and objectives that are not covered by the above questions.
3. Please identify agency-wide issues that should be addressed by NSF to help improve the program's performance.

A very important but neglected area is the relationship between academia and industry. This includes the REU program and every other area of chemistry. The relationship has deteriorated over the decades to the detriment of both groups. Mechanisms for improving the situation might well come under the purview of the NSF. We suggest a committee be formed to investigate and make recommendations.

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.

The agency provided a suitable batch of proposals and good overview of activities during the 2013-2015 period.

Depending on the feasibility, it would be good to have the following information for the COV process:

- 1) An overview of the number of submissions from each state since the COV is asked to evaluate the distribution of awards across the US.
- 2) Summative data on the institutional and demographic make-up of the reviewers. As much as possible, the reviewers should be a reflection of the various types of institutions and diversity of scientists that the agency is hoping to support. It would be good to see if the agency is already doing this.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Major Chemical Research Instrumentation and Facilities (INSTR)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>The MRI program relies primarily on panels. The available data showed that discussions in panels were useful in refining the evaluations that reviewers prepared in advance. The summary data shows that more mail (ad hoc) reviews were obtained in 2014 and 2015 than in 2013. The "FY 2015 Panel Memo" states that ad hoc reviews were solicited for some of the more expensive proposals and for development proposals. This is a wise decision.</p> <p>Virtual panels permit discussion of smaller groups of related proposals by experts to an extent that would not be possible if these were grouped together in a larger more heterogeneous set for discussion in an on-site panel. Virtual panels can permit more time to be allocated to individual proposals. However, there was a difference of opinion on the COV about the value of virtual panels in this program.</p> <p>On the panels there was an appropriate mix of people from PUI and PhD granting institutions, which is important because about half of the proposals were from PUIs.</p> <p>Data Source: data provided</p>	<p>Yes</p>

<p>2. Are both merit review criteria addressed</p> <p>In individual reviews? YES</p> <p>In panel summaries? YES</p> <p>In Program Officer review analyses? YES</p> <p>Comments:</p> <p>Panels and program officers are consistent in addressing broader impacts. Individual reviews usually do so, but maybe not always.</p> <p>Panel summaries sometimes included issues that were not mentioned in any of the individual reviews. This reflects discussion in the panel that helps to inform decisions.</p> <p>Related to 2013 COV question – Are panels unduly impressed by 'over-the-top' suggestions for broader impact?</p> <p>Response: Within the MRI proposals broader impact often involves making the instrumentation available to users from other schools and sometimes high school. These seem to be appropriate, but not excessive expectations.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>Most reviewers do careful and conscientious reviews, but some do not. The panel mechanism provides opportunity for discussion and clarification. When comments from one reviewer differ from those of another, discussion is useful.</p> <p>Constructive criticism is crucial for feedback to PIs whose proposal is not funded. It might be helpful to the overall review process if the program officer made suggestions for improvement of reviews when they see that a reviewer is less thorough in their evaluations.</p> <p>It could be helpful to request that reviewers limit the fraction of proposals to which E or V scores are given.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>Panels are conscientious in documenting the basis for recommendations. When there are differences of opinion, the program officers can follow up. This is important primarily for proposals that are near the cut-off for funding.</p> <p>Data Source: Jackets</p>	<p>yes</p>
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>Rationales are provided. Some of this rationale may not be communicated to the PI in the letters that are sent out.</p> <p>Data Source: Jackets</p>	<p>yes</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>Documentation is sufficient when we see the full process, which is carefully done. It may be less clear to a PI. Where needed, the PI has the option to speak with the program officer but is unlikely to do this. In some cases the panel discussion was more or less enthusiastic than the scores implied. In those cases it could be helpful to the PI in understanding the final decision if the letter grades were revised so that the PI is not confused by the final decision.</p> <p>Data Source: Jackets</p>	

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

Merit review procedures involving panel plus outside reviewers is generally strong.

When a reviewer gives an overall evaluation it is not always clear how the components of intellectual merit and broader impact are weighted.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>The quality of comments indicates that reviewers had appropriate expertise. In this program, there was an appropriate balance of reviewers from PUI and PhD institutions, and a range of schools within each category.</p> <p>Data Source: Jackets</p>	yes
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>It's hard to judge from the ejackets. The Program Officers' analyses and comments indicate careful attention to COI. This program appears to have done an outstanding job in avoiding COIs.</p> <p>Data Source: Jackets</p>	yes
<p>3. Additional comments on reviewer selection:</p> <p>There is an appropriate mix of reviewers from PUI and PhD granting institutions. PUI panelists represent institutions from a mix of PUI-type institutions. Panels seem to understand the differences in expectations for MRI proposal requests from PUI and PhD institutions.</p>	

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.

Comments:

This seems to be an extraordinarily well-managed program. The program officer analysis provided detailed information. They put substantial effort into addressing questions raised by the panel and in organizing co-funding by multiple programs. They negotiated with PIs concerning details of the budget, which permitted funding a larger number of proposals. The program officer recognizes the importance of broader impacts, particularly for some of the PUI proposals. They are handling a heavy load.

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

Comments:

It is difficult to find fault here. The MRI program responds to the mix of proposals that is sent to them, which seems appropriate. However, there is an unfortunate lack of proposal pressure in instrumentation development. High risk proposals are noticeably absent. Development proposals were a small fraction of the mix but were given due consideration. The groupings into panels have changed over the past several years in response to proposal pressure, which is appropriate. Improving technology that permits virtual panels that focus on sets of 5 to 19 related proposals provides the opportunity to select reviewers with specialized expertise. This seems preferable to having large heterogeneous panels.

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

Comments:

The Program Officer analysis documents indicated a desire to have a balanced portfolio of awards. The balance was across areas such as gender, race, ethnicity, geography, type of institution, type of research, new and early-career investigators, and type of equipment.

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

Comments:

The 2013 COV had recommended the use of virtual panels for all but the "subgroups with the largest numbers of proposals".

Response: This recommendation has been followed. It would be interesting to have PO comments on how well they feel this has worked. The COV members are not in agreement on this point, based heavily on their own experience in panels. The divergence of experience indicates the importance of the PO role in managing the virtual panel.

The 2013 COV asked about accountability related to broader impact. Has the division reviewed progress reports to compare outcomes related to broader impact with the statements in the proposal? The chemistry community still does not have a clear sense of what is expected in the 'broader impact' category and how to evaluate broader impact in their reviews.

CRIF was eliminated as a separate program with its own deadline and folded into the MRI program. The Division still provides additional money to supplement the MRI funding, which is essential given the extent to which chemistry research is dependent on instrumentation. The COV strongly supports continuation of this Chemistry Division funding support, given the fact that CRIF no longer exists.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

- How much funding should be allocated to supplement MRI compared with the total chemistry division budget? Essentially all chemistry research is heavily dependent on instrumentation. Increased funding would permit augmenting the overall portfolio. The COV encourages the Division to advocate the Foundation for an increase in the overall MRI budget.
- The program is funding work at a range of institutions.
- New PIs had success rates that were only a bit lower than the overall success rates.
- A number of awards were co-funded with other entities within NSF.
- Geographic distribution of the awards appears fine and representative of the submissions.
- In FY15, 4-year institutions had an exceptionally low funding rate (1/22) as compared to FY13 (3/18) and FY14 (6/22), relative to other PUI (MS schools) or PhD institutions.
- Underrepresented groups are represented in the portfolio (women – about 27%; URM – about 24%) at levels commensurate with their representation in the discipline.

OTHER TOPICS

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

There is great need and opportunity for support of mid-scale (\$1M – 5M) instrumentation development programs in the chemical sciences. Proposals at this level will likely be interdisciplinary, and many will be chemistry-centric, yet there is no Chemistry program covering this level, even though other MPS areas do have activity and MRI calls for proposals at this level of scope.

The program is well distributed. There were a couple of proposals from PUIs where it appeared that the instrumentation was funded more on the positive aspects of having students participate in research projects than on the intellectual merit of the research projects proposed by the investigators. In both cases, these were very modest requests (less than \$50K) so the decision is understandable. However, reviewers should appreciate that high quality research can be done at PUIs and that high quality, published research ought to be a primary goal for programs awarded instrumentation grants.

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

The Program Officers are doing an amazing job allocating the limited resources available. The lack of proposal pressure for instrumentation development is surprising. NSF leadership in chemistry could be much strengthened by better showcasing of this area in terms of accomplishments and opportunities.

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

Instrumentation is crucial to all aspects of chemical research. The highest priority should be to increase the resources available. We strongly support the Chemistry Division continuing to augment MRI funding with CRIF funding. Even with the CRIF contribution added to MRI funds, there are insufficient funds to support all deserving proposals.

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

The uncertainty in how and the extent to which previous CRIF funding will be replaced is a significant concern. The Chemistry Division is currently supplementing MRI awards, but one must ask if instrumentation acquisition and development is on a firm footing.

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

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Macromolecular, Supramolecular and Nanochemistry (MSN)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate?</p> <p>Comments:</p> <p>MSN used a combined method of panels (onsite + virtual) and ad hoc mail reviews, which is balanced and appropriate. We recommend that proposals be reviewed as often as possible within a panel (with mail-in ad hoc reviews to provide additional expertise as necessary).</p> <p>Data Source: information provided by program</p>	Yes
<p>2. Are both merit review criteria addressed</p> <p style="padding-left: 40px;">In individual reviews?</p> <p style="padding-left: 40px;">In panel summaries?</p> <p style="padding-left: 40px;">In Program Officer review analyses?</p> <p>Comments:</p> <p>Individual reviews: Most reviewers provided a more substantive analysis for the Intellectual Merits section in comparison to the Broader Impacts section. In addition, there was much more variability in what reviewers looked for in the Broader Impacts. We noticed that foreign reviewers tended to rate the proposals less favorably overall, and to overlook the Broader Impacts review criteria.</p>	Yes

<p>Panel summaries: Panel members did a great job integrating the ad hoc reviews and captured a balanced discussion. For declined proposals, PIs were provided suggestions for how to improve their proposal for the next submission. However, there was some variability in the thoroughness of this feedback from proposal to proposal.</p> <p>Review analyses: MSN POs should be applauded for their diligence in providing detailed analyses to justify award and declination decisions. Details of prior funding analysis, citations, and PI history were provided in many cases to justify an award decision. However, MSN should consider whether more of the factors discussed in the review analysis could be relayed to the PI in the written PO comments.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals?</p> <p>Comments:</p> <p>Most reviewers provided substantive comments to justify their review score for Intellectual Merits, but less so for evaluation of the Broader Impacts. For certain awarded proposals, some the reviews were too concise and did not provide substantial feedback. In these cases, however, there were enough substantive and longer reviews to mitigate the effects of a non-review.</p> <p>Data Source: Jackets</p>	Yes
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)?</p> <p>Comments:</p> <p>Overall, the Panel Summaries successfully captured the main comments of the ad hoc reviews and often went well beyond in their discussion and analysis of the proposed work. Such thorough analysis likely helped the POs construct their detailed review analyses.</p> <p>Data Source: Jackets</p>	Yes

<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision?</p> <p>[Note: Documentation in the jacket usually includes a context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), program officer review analysis, and staff diary notes.]</p> <p>Comments:</p> <p>For most proposals, the rationale for the award/decline decision was commensurate with the reviews. There were a few awarded proposals, however, in which the PO’s decision to fund the proposal did not seem consistent with the written recommendations of the panel or ad hoc reviewers. For example, there was a case where the proposal received a low ranking from panel members (tier 3), while the PO recommended funding with an adjusted budget. We reasoned that this might be from the considerations of balancing the portfolio, but that was not made clear in the written review analysis.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision?</p> <p>[Note: Documentation to PI usually includes context statement, individual reviews, panel summary (if applicable), site visit reports (if applicable), and, if not otherwise provided in the panel summary, an explanation from the program officer (written in the PO Comments field or emailed with a copy in the jacket, or telephoned with a diary note in the jacket) of the basis for a declination.]</p> <p>Comments:</p> <p>The individual reviews and panel summaries frequently provide a reasonable rationale for the funding decision. However, there was some variability in the effectiveness of the PO comments. Some POs did an outstanding job of providing useful summary information, and we recommend that standardization of this practice by all POs would strengthen the MSN review process.</p> <p>It appears that proposal ranking was changed from “tiers” to “priority” in 2015, with PIs being notified that their proposal was either ND (not discussed), low priority, medium priority, or high priority. The COV reviewed this change favorably.</p> <p>Data Source: Jackets</p>	<p>Yes</p>

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

The merit review process appears to be generally effective; however, there were some discrepancies between PO funding decisions and the panel/review recommendations. Justification could have been clearer in the review analysis (e.g., an instance of balancing portfolio).

Some panel summaries did not contribute information beyond that found in the ad hoc reviews.

The COV notes that MSN handles a fairly large number of proposals, and given this breadth, the POs handled the challenges relatively well.

POs are extremely careful and attentive in their detailed analysis. They should be commended.

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications?</p> <p>Comments:</p> <p>The POs assembled panels and solicited ad hoc reviewers with a good breadth and depth of representation across different institutions. The reviewers were balanced in expertise and were at different stages in their careers. Most, if not all, of the proposals submitted from a PI at a PUI had at least one reviewer who was also from a PUI.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>2. Did the program recognize and resolve conflicts of interest when appropriate?</p> <p>Comments:</p> <p>NSF has a high standard on COI in general, and the POs appear to be diligent in maintaining the standard.</p> <p>Data Source: Jackets</p>	<p>Yes</p>
<p>3. Additional comments on reviewer selection:</p> <p>The POs sometimes selected ad hoc reviewers from the PI's recommended list, as well as other experts in the subject area; the balance is good. The selection of ad hoc reviewers was properly documented. The selected reviewers cover a broad range of expertise.</p>	

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

MANAGEMENT OF THE PROGRAM UNDER REVIEW
<p>1. Management of the program.</p> <p>Comments:</p> <p>The POs of MSN have done an effective job managing the program, from soliciting panel and ad hoc reviewers to the final award decisions. The MSN program seems to have a fairly large number of submissions (~270), which could make it difficult to manage and could be why there is a large number of POs.</p> <p>There was evidence of co-funding for many of the proposals, indicating that the program officers within MSN are reaching out to other entities as appropriate.</p>
<p>2. Responsiveness of the program to emerging research and education opportunities.</p> <p>Comments:</p> <p>Good responsiveness overall. One example is that the program highlighted sustainable chemistry in the program description, which is closely related to emerging global issues.</p> <p>The program description of MSN is very clear and shows the delineation from other programs—this should be commended. The program description also encouraged submissions related to the chemistry of nitrogen, phosphorus, and water in the nexus food, an NSF-wide initiative.</p>
<p>3. Program planning and prioritization process (internal and external) that guided the development of the portfolio.</p> <p>Comments:</p> <p>The program is funding a range of work within the broad scope of MSN fields. 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. That said, the PO review analysis documents rarely seemed to comment on whether these factors were used in making a final decision.</p>
<p>4. Responsiveness of program to previous COV comments and recommendations.</p> <p>Comments:</p> <p>There is no previous COV comments or recommendations directed to MSN.</p>

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

Please comment on portfolio balance considering balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities.

Overall the program has a well-balanced portfolio in most aspects. Specific points are noted below.

Inter- and multi-disciplinary projects: MSN is involved with a relatively high number of inter-disciplinary projects with other programs in CHE and with other divisions, with frequent joint co-funding efforts.

Women and under-represented minorities: The success rate of URMs was much lower than the overall success rate. The numbers (total submission, number of awardees, and percentage) increased every year, which is seen as a sign of positive effort of the POs on balancing the portfolio. Women have success rates almost identical to the overall success rate of proposals with the program.

New PI and early-career PIs: New PIs have a slightly lower acceptance percentage than the average (8-10% lower than established PIs), although the number increased each year over the three-year period for which data was provided. This could be tracked back to inexperience in proposal writing or lack of preliminary results. Efforts to reach out to URMs and new PIs with workshops on effective proposal writing appear warranted.

Primarily Undergraduate Institutions: The number of submissions from 4-year institutions is disappointingly small. The success rate of proposals from Masters institutions is especially low over the past two years (25.0%, 11.1%, and 6.7% over the past three years, respectively). We were provided information on several RUI proposals, and the rationale for the decision was well documented and justifiable. Hence, this audience might also benefit from workshops on effective proposal writing.

The geographic balance of awards seemed appropriate to the geographic submission of proposals.

OTHER TOPICS

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

Finding good rotators that can stay for many years will provide additional stability to the program.

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

The funded awards fall within the research areas of the program description.

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

The use of a review response template with required fields (covering the suggested NSF review elements) could improve the consistency and quality of the written reviews.

It could be useful for POs to release summary statements including the individual reviews and panel summaries before the PI is notified of the award/decline decision. Timely feedback is important for PIs who seek to resubmit revised proposals that were not funded during the initial submission.

It could be useful for POs to have a system for evaluating/ranking strong and poor reviewers.

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.

The ejacket website is cumbersome and inconvenient to navigate. It would be nice if it was easier to toggle directly between components of the application.

INTEGRITY AND EFFICIENCY OF THE PROGRAM'S PROCESSES AND MANAGEMENT

Chemical Synthesis (SYN)

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, and withdrawals) that were *completed within the past three 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
<p>1. Are the review methods (for example, panel, ad hoc, site visits) appropriate? In part.</p> <p>Comments:</p> <p>In general, the review process conducted by panelists, and augmented with mail-in ad hoc reviews, is considered very effective. The panel reviews and summaries substantively assess the intellectual merit and broader impacts. In-person panels appear to give more unified results, and the COV noticed adjustments between the individual reviews and the panel summary. The review process involving purely mail-in ad hoc reviews (proposals not reviewed in panel), seems less effective; the proposals do not receive a thorough discussion of the project. For example, a CAREER proposal (from 2013) was not reviewed by a panel and only had 3 reviews, one of which was very minimal with absolutely no description. This is problematic.</p> <p>In addition, it is noted that for proposals that are "not discussed," the true strengths and weaknesses of the proposal are not clearly articulated to the PI (although it is realized that this is the case only for the lowest ranked proposals).</p> <p>The general assessment is that every effort should be made to review proposals by a panel, as this results in a much more effective review process. It was not clear that the advantage of having experts review by mail outweighed the disadvantage of not having a panel discussion. When a proposal is reviewed purely by mail using ad hoc reviewers, it puts the onus on the PO to synthesize comments and weigh the funding priority of the proposal. The ad hoc</p>	

<p>reviews are usually very effective, and the summaries or review analysis do an excellent job of pulling together the perceptions.</p> <p>Data Source: data provided</p>	
<p>2. Are both merit review criteria addressed</p> <p>In individual reviews? Yes</p> <p>In panel summaries? Yes</p> <p>In Program Officer review analyses? Yes</p> <p>Comments:</p> <p>For the most part, the individual reviews focused more on the Intellectual Merit than the Broader Impact, although at least a sentence or two considering the Broader Impacts of a given proposal were provided. There is a sense that some reviewers do not appropriately value the Broader Impacts for standard research proposals. For CAREER proposals, both were weighed more equally because of the explicit teaching component of this award mechanism.</p> <p>The definition of broader impacts used in the individual reviews is very broad, ranging from whether the chemistry is going to be disseminated, to outreach to under-represented groups. A consistency of understanding of Broader Impacts is essential to making this evaluation useful.</p> <p>The panel summaries were much more consistent in providing an overview of the Broader Impacts, as were the PO Review Analyses. In one case, the DGA (Division of Grants and Agreements) felt that a PO Review Analysis did not adequately comment on the Broader Impacts. This was noted and addressed appropriately in a diary comment.</p> <p>Data Source: Jackets</p>	
<p>3. Do the individual reviewers giving written reviews provide substantive comments to explain their assessment of the proposals? Yes</p> <p>Comments:</p> <p>Overall, the individual reviewers were very conscientious in their written reviews, providing substantive comments discussing the strengths and weaknesses of the proposal. It is noted that the styles of the individual panel reviews vary substantially, with some reviewers writing long narrative paragraphs, and others writing concise bulleted points. Although the NSF provides a “template” and suggests key review elements that should be considered, the actual template for the responses is not very specific. The</p>	

<p>NSF could consider providing a more specific template, where the review elements are provided as bullet points to be addressed by the reviewer.</p> <p>There were a minority of reviewers who did NOT provide substantive comments, and other reviews ignore all but the science. This could be problematic, especially if the proposal is not reviewed in a panel and therefore no panel summary is provided. Reviewers should be encouraged to provide substantial reviews (and again, this could be encouraged by a better review template).</p> <p>Data Source: Jackets</p>	
<p>4. Do the panel summaries provide the rationale for the panel consensus (or reasons consensus was not reached)? Yes</p> <p>Comments:</p> <p>The panel summaries did a good job of capturing the consensus of the individual panel reviews. In cases without complete consensus, the source of the disagreement was noted, as well as whether or not this was perceived as a major or minor disagreement. It is clear that panel discussion was required to achieve consensus on many of the proposals.</p> <p>Data Source: Jackets</p>	
<p>5. Does the documentation in the jacket provide the rationale for the award/decline decision? Yes</p> <p>Comments:</p> <p>The Panel Summary, Review Analysis, PO comments, and other documentation provided useful insight regarding the award/decline decision. The Review Analysis was particularly helpful in understanding how the decision was made, particularly for the “tier 2” or “medium priority proposals.” It is important for the Program Officer to add notes to the PI for declined proposals on what may be necessary for success in that division or to submit to other divisions.</p> <p>Data Source: Jackets</p>	
<p>6. Does the documentation to the PI provide the rationale for the award/decline decision? Yes</p> <p>Comments:</p>	

<p>The PIs are provided the individual panel review comments and the panel summaries. It appears that nearly all (if not all) of the time, this information was identical to the panel review comments and panel summaries coming directly out of the review process. For the most part, the panel review summaries provide the PI with good rationale for the award/decline decision; however, for proposals ranked as “medium priority,” the PI’s feedback may seem more ambiguous with respect to how it influences the award/decline decision. There were times when the reviews focused on aspects that were not the primary focus of the PI, but these were well justified and explained in detail in the reviews and PO communications.</p> <p>It is important for the Program Officer to add notes to the PI on declined proposals on what may be necessary for future success in SYN or to submit to other programs, Divisions, etc.</p> <p>NOTE: Many PIs do not get panel reviews/panel summaries in a timely fashion. This can be challenging for PIs with proposals ranked as “medium priority,” who need to consider submitting a revised proposal. Some COV members suggest that it would be better to give panel summaries at an earlier time in the process before the funding decision is announced.</p> <p>Data Source: Jackets</p>	
<p>7. Additional comments on the quality and effectiveness of the program’s use of merit review process:</p> <p>The program has developed a good process for merit review. Some COV members think that it could be helpful to have panels devoted to reviewing RUI proposals so that these proposals are considered relative to their peers, rather than PIs at institutions with different expectations/resources. This would result in better overall process of truly meritorious RUI proposals. In some cases, funding of RUI proposals is at the discretion of the PO because in some programs, it is rare for a RUI to be considered a “high priority” proposal.</p> <p>For the RUI program, there were a number of disparate bases for review. Providing opportunities for undergraduate research at times seemed to be sufficient for strongly positive statements, even when the research was not praised, while at other times, the research got the praise, while the undergraduate involvement was at best secondary.</p> <p>Because the E, V, G, F, etc. rating includes an interpretive meaning that may not be analytically valid, some COV members think that it might be better to move to a numerical rating system. In a few instances (see above), proposals were rated high according to this system. However, the POs (rightfully so) recognized that the E ratings were at times overestimated as the written evaluation did not match the rating. As an NSF-funded PI this observation is reassuring (i.e., overestimated proposals do not get funded).</p>	

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
<p>1. Did the program make use of reviewers having appropriate expertise and/or qualifications? Yes</p> <p>Comments:</p> <p>The panels were a good mix of chemists with appropriate expertise and at different career stages. The panels primarily consisted of researchers at PhD granting institutions, but also had representative members from PUIs or MS-granting universities. There appears to be a good effort to have representation from both genders.</p> <p>It was clear from the jackets that the POs went to great pains to have appropriate chemical expertise represented on the panels. Some specialties were better covered than others, but it seemed that each panel had at least one person with in-depth knowledge of the field. It should be a priority to represent appropriate expertise on panels themselves rather than through ad hoc, mail in reviews.</p> <p>Data Source: Jackets</p>	
<p>2. Did the program recognize and resolve conflicts of interest when appropriate? Yes</p> <p>Comments:</p> <p>There were no cases in which there was conflict of interest on the panels, and very few cases in which actual conflicts of interest were discussed.</p> <p>Data Source: Jackets</p>	
<p>3. Additional comments on reviewer selection:</p> <p>There were a few panels that had two reviewers from the same university, which is viewed as non-ideal. In these cases, however, the PO made a special note to discuss why it was necessary. Typically, it was deemed necessary due to lack of availability of other reviewers with the appropriate expertise. However, it is surprising that program truly could not find reviewers from different</p>	

institutions with appropriate expertise.

It should be considered whether to eliminate reviews that are not suitably useful and do not give enough details for PIs to revise the proposal. As mentioned above, perhaps a template for the reviewers may be appropriate.

Some panels, such as RUI, seemed to have disparate understandings of the goals of the program. Whether this was a problem in reviewer selection or in training at the panel is impossible to say.

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.

Comments:

The program seems well managed overall, and it is clear that there is great effort to provide rationale for the basis of the decisions.

Some COV members think that it would be good for the program to send summary statements to the PI ahead of the award/decline decision process (i.e., shortly after panel meeting instead of months later).

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

Comments:

Overall, the program seems responsive to emerging research and educational opportunities. However, some reviewers' comments on Broader Impacts suggest that they are not aware of emerging and interesting education opportunities. The program could also consider whether to use specific initiatives to entice new opportunities in education, such as on line courses.

There was much discussion of the innovative nature of the research. The discussion of broader impacts in terms of educational opportunities often was focused as much on the institution as on the PI. At times the PI could claim involvement with or support of an institutional initiative, and at other times, the PI was the initiator. It was not clear from some reviews that there was a difference in value added.

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

Comments:

From the last COV, there were questions of how to sort proposals between synthesis and catalysis, with a desire to identify grand challenges in synthesis that don't involve catalysis. This separation of synthesis and catalysis seems somewhat contrived: many strong synthesis programs have elements of catalysis. It is good to continue to have POs who bridge synthesis and catalysis, rather than attempting to completely separate these disciplines.

There were very few female PIs and very few proposals from small institutions that were funded. It may well be that the Synthesis program is not an appropriate target for small research programs, but NSF needs to find a way to support research at smaller institutions, since a disproportionate number of graduate students come from such institutions.

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

Comments:

The program appears responsive to addressing the comments from the prior COV report.

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

Programs should provide materials to the COV regarding portfolio goals and can insert specific targeted questions about their portfolios. (Some dimensions of portfolio balance to consider include: balance across disciplines and sub-disciplines, award size and duration, awards to new and early-career investigators, geographical distribution of awards, awards to different types of institutions, innovative/potentially transformative projects, projects with elements of risk, inter- and multi-disciplinary projects, projects that integrate research and education, participation of groups that are under-represented in science and engineering, and projects that are relevant to agency mission or national priorities).

The SYN portfolio of funded proposals seems reasonably balanced, including PIs at research institutions as well as PUIs. It is noted that there were no funded GOALI proposals in the SYN program, and that the only EAGER application was returned without review. Considering the awarded subset of jackets that were reviewed, there were two that can be categorized squarely as total synthesis, two that were a combination of methods and synthesis, three that were methods, one methods with applications to carbohydrates, and one methods with applications to materials. This seems like a good balance. Of this cohort, two awards were made to PIs at PUIs. It was clear that at times, slightly lower-priority proposals (in terms of the panel review) were funded in an effort to generate a balanced portfolio, particularly with respect to the PUI investigators and gender. Similar decisions were also made to fund research areas that were viewed as underrepresented in US research programs, but that were viewed to have significant broader impacts. Overall, it appears that the highly meritorious proposals were funded, and the POs used discretion to make funding decisions of "second tier" or "medium priority" proposals to help balance the portfolio. This seems reasonable.

The SYN program has received a total of 515 proposals over the last three years, of which 149 were funded for a funding rate of 28.9%. This number is in-line with the Division of Chemistry fund rate, which is 26.2% (1436 awards/5474 submitted). These awards are appropriate in terms of total dollars (\$141,700/year) and duration (3.0 years). These numbers are slightly below the total dollar amount (\$162,800/year), but in-line with duration (3.1 years) for Division averages. SYN includes a modest number of awards that are funded through other directorates (MPS-CHE-CAT (main) and MPS-CHE-Projects, MPS-OMA, and MPS-CHE-CLP among others) for a total funds-out of \$151.1 (K per year) and funds-in of \$3,711.0 (K per year). The portfolio does have a reasonable national award distribution with funded states on the west coast (CA, OR), southwest (TX, OK), midwest (MN, WI, IL, IN, IA), southeast (LA, GA, FL, NC) and northeast (NY, MA, PA). However, there is a neglected section of the country to which no SYN-funded grants have been awarded especially in the plains states (ND, SD, KS), parts of the west (MT, NV, WY), southeast (MS, AL), and AK and HI. It is recommended that the program targets these states better, including finding a more effective solicitation strategy for regions with a poor participation rate. Of the awards made, the majority have gone to Research Intensive (Top 100) PhD institutions (103/149 awards = 69.1%) with Masters Institutions (8/149 = 5.4%), Business, State and Local Foreign (BSLFO, 5/149 = 3.4%), and 4 year schools (3/149 = 2.0%) rounding out the top. In general, these numbers reflect the percentage of submitted proposals by these types of institutions, viz.: Research Intensive Ph.D., 274/515 = 53.2%; BSLFO, Masters, 46/515 = 8.9%; 24/515 = 4.7%, 4 year, 14/515 = 2.7%. More efforts should be made to increase the number of submitted/funded proposals to these non-PhD institutions. New investigators are slightly underrepresented, which is demonstrated by the 17.0-17.6% fund rate of SYN proposals that are in the new or new involvement PIs category compared to the overall SYN rate of 28.9% and considering that 204/515 = 39.6% of proposals are from new or new involvement PIs. The fund rate of women (27.2%) and underrepresented minorities receiving SYN awards (26.3%) is mostly in-line with the SYN overall fund rate of 28.9%, the Division fund rate for women and minorities (26.2 and 21.4%, respectively) and the overall Division fund rate of 26.2%.

OTHER TOPICS

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

None are noted.

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

The awarded proposals are appropriate in meeting program-specific goals and objectives, covering areas including the discovery of new synthetic methods, target-oriented synthesis, and synthesis of novel organic, organometallic, and inorganic structures. Although there is a stated interest in funding research in sustainable chemistry, it seems that relatively few proposals in SYN were funded under the SusChEM program. It is also noted that more of the awarded proposals focused on elements of organic synthesis and organic reaction development rather than organometallic/inorganic synthesis, but this is somewhat representative of the distribution of the research areas of the submitted proposals.

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

If the mission is to fund transformative research, the funding levels for individual grants may not be commensurate with achieving that goal.

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.

The EJacket website is very cumbersome, requiring far too many "mouse clicks" to review a given proposal. It would be great to click one button, and have the project summary, reviews, panel summary, and review analysis in one document. It was hard to get back to the panel home page.

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SIGNATURE BLOCK:



For the 2016 Division of Chemistry COV
Dr. Sharon Hammes-Schiffer
Chair