Update to the CHE Response to the 2013 Report of the Committee of Visitors April 2014

The Division of Chemistry (CHE) wishes to thank the members of the 2013 COV panel for their time and effort on the review of the activities of the Division. We are especially grateful to Dr. Joseph Francisco for his exemplary leadership during the COV process, resulting in the timely completion of the final report.

We appreciate the thorough review and the realistic, actionable recommendations. We are delighted that the COV panel recognized the Division's devotion to a thoughtful and fair review process and are pleased with the high marks the Division received. In the following, we respond to the specific recommendations in the same order as presented in the executive summary of the report. If deemed necessary for clarification, passages from the full report are quoted.

"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 PI's.*** *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."*

"*…establishing a database of reviewers"*
The Division took leadership in evaluating commercial reviewer database software, beginning in fiscal year 2010 (FY10). Note that the existing database is not searchable, but does allow program directors to view the NSF review record of individual reviewers. The Division's initial effort resulted in a request for bids for the acquisition and installation of a more advanced database. Most likely driven by NSF's requirements on security and confidentiality, no bid was deemed acceptable by NSF; in a second round, no bids were received. CHE revisited the issue in late FY12, with continuing efforts in FY13. The issue was elevated to a higher level. NSF's Chief Information Officer is strongly supportive of such a database, cross-linking with NSF's existing electronic business applications. The cost for this endeavor is considerable and requires approval and buy-in at all levels. Despite the current fiscal uncertainty, CHE is optimistic that such a database will be established on an NSF-wide level, but establishing it may take some time.

Update April 2014
Since the Foundation has not yet implemented an NSF-wide database, the Division developed three interim solutions. Firstly, the Division collected individual program director databases and combined them into one Excel file. About a decade ago, the

Division had hired a contractor to develop a searchable database that was rendered inoperable in 2012 when the Foundation moved to Windows 7. The Division retrieved the data and ported them into Excel format, where they were combined with individual program director reviewer data. This database now contains more than 5,000 records, including keywords describing the reviewers' expertise. It was ported to Sharepoint where it is easily accessible to all CHE members.

Secondly, CHE developed a survey that will be linked from our website. This survey form asks community members to volunteer their services as reviewers. The future reviewer enters his/her own information, including optional demographic data. The reviewer selects programs that s/he would like to review, and describes his/her expertise with up to ten keywords. This survey went through OMB clearance and is now ready for posting on the CHE website. We anticipate this to be completed by the end of May 2014.

Thirdly, the Division committed funds to join in an effort that is spearheaded by the Engineering Directorate (ENG). ENG developed a tool ("PRIM") that is equivalent to the eCorrespondence tool in eJacket. The program director can select reviewers for panels and ad hoc review and ask them to specify their expertise by check-marking boxes. These text items will be under full control of chemistry. Once a reviewer has been asked to enter his/her information, the record remains in the database so that over time a new database is being built. The database will be pre-populated with the records from the two databases (Sharepoint and Reviewer Survey) as described above. This database will allow the program director to assign reviewers to proposals in panels, and conduct all necessary correspondence. However, while these records are permanent, they will not be linked to the jacket in eJacket. The next release of PRIM will implement this feature. In order to allow for this step in the development, CHE committed funds to support the effort. Implementation is expected in FY15.

"*… developing mechanisms for educating the reviewer pool"*

CHE strives for continued, clear communication with the principal investigator (PI) community. Given the recent federal travel restrictions, we have reached out to the community by offering virtual participation at chemistry department meetings. We advertise this opportunity in our Newsletters, at panels, on outreach trips, and in one-on-one conversations with community members. Surprisingly, the interest by academic departments has been rather small (about 5 requests in calendar year 2012), but we will continue our efforts to communicate this opportunity. We use these venues to communicate priority research areas, provide coaching, mentoring and training in reviewing and writing proposals, conduct special training sessions for early career investigators, and answer specific questions, such as the recurring one on the balance of Broader Impacts versus Intellectual Merit.

Update April 2014

CHE created a divisional working group that is charged with developing materials for educating the reviewer community. The content developed by this working group will be disseminated by the divisional Outreach Working Group. We anticipate that these efforts will continue through fiscal year 2015.

"***…****transparency in identification and development of priority research areas and clarification of broader impacts.* ***"***

A recent task force of the National Science Board was charged to review and revise the NSF Broader Impacts criterion that continues to cause misperceptions in the community.

The task force made specific recommendations that were implemented in the latest Grant Proposal Guide, and added to the reviewer template.

"*...evaluation of the broader impact component should be consistent across programs of the Division"*
NSF does not provide guidance to the reviewer community on the relative weight of Broader Impacts and Intellectual Merit, which leads to a wide spectrum of reviewer responses. CHE program directors very carefully analyze the merits of a proposal with regard to both criteria. While proposal outcomes are largely determined by reviewer feedback, program directors also consider portfolio balance in their recommendations. The convolution of both aspects appears to have raised the perception by COV members that the relative weight of both criteria was inconsistently applied across programs. The Division will enhance its efforts to more consistently document this process.

"...composition of review panels is as diverse as possible"
In the full version of the report, the COV recommended that the identity of panelists be made public as is the practice at the NIH. The rationale for the recommendation was two-fold – allow the PI community to be assured that the correct expertise is present at the review panel, and assure that conflicts of interest (COI) are addressed.

The issue raised by the COV pertains to NSF as a whole, and the change of NSF policies is not under the purview of CHE. It is NSF's policy to keep the review process strictly confidential as NSF believes that only anonymous merit review ensures reviewers' candor.

In addition, we would like to reaffirm that COIs are taken very seriously at NSF and every proposal is thoroughly screened for potential conflicts before it is released to a reviewer or panelist. Reviewers and panelists are asked to disclose additional conflicts that cannot be identified by NSF (such as personal friendships or inadvertent omissions in the list of collaborators provided by the PI). Every reviewer has to sign a conflict-of-interest and confidentiality form before being allowed access to the proposal.

NSF panels are covered under the Federal Advisory Committee Act (FACA), and the identity of reviewers in the annual pool is disclosed on a public website (see http://fido.gov/facadatabase/).

For comparison, NIH's portfolio is mission-oriented leading to greater homogeneity in the proposal and reviewer pool, and allowing for larger panels. The large panel size coupled with term membership help to conceal the identity of individual comments. The term system, however, has led to racial bias and NIH is in the process of reviewing its practice.

Lastly, the COV recommended that young investigators be included in the review process. We would like to emphasize that we do so whenever possible, as we regard panel service and ad-hoc review as a learning experience to improve grantsmanship and as a career-building opportunity. However, we are mindful to only include young investigators who have sufficient experience to serve on a panel.

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

The COV's concern was lack of continuity in programs staffed by rotating program directors (PDs). Currently, the Division has about 60% permanent and 40% rotating PDs, which we consider a healthy balance. While our permanent PDs provide the desired continuity, the rotating PDs bring in fresh ideas and are more closely in touch with the issues concerning researchers in the scientific community. Nevertheless, we agree with the COV that some of the programs were subject to frequent personnel changes due to difficulties in hiring and delays in on-boarding new rotators. Rotators under consideration for hiring cannot have any proposal in "pending" status, or submit new proposals. The Division has implemented a working group that is charged with developing a robust plan that merges continuity and scientific breadth, with the additional constraint that the Point of Contact (POC) or Program Lead be a permanent staff member. The plan will also address succession planning.

Update April 2014
The Division has staffed all programs with permanent program directors as program leads. In order to achieve this goal, some program directors had to change their assignments; in some cases after many years of service in a specific program, providing new opportunities for program directors and preventing burn-out. In addition, the Division is currently in the process of interviewing candidates for rotators. The first wave of interviews is being conducted in April/May of 2014 for candidates with a possible start date of fall 2014. A second wave of interviews will be conducted in Fall 2014, for a start date of fall 2015.

"Recommendation #3: Increase the efficiency of operations and the number of Program Officers to improve program management. *The COV recommends that the Division be given positions for additional personnel in order to decrease the workload currently imposed on Division staff, to ensure adequate oversight and program management, and to allow progress on new and existing programs and projects."*

We are delighted about this recommendation as we wholeheartedly agree. In fact, every year when the Divisional workforce analysis is undertaken, we request additional program director positions. Unfortunately, they are available neither to us nor to MPS, and this recommendation is out of our hands to implement.

"Recommendation #4: Reevaluate the distinction between the catalysis and synthesis programs and investigate best ways to categorize the programs in these areas."

We have established an internal working group to tackle this issue. Our first step is to mine data. We are in the process of identifying proposals where the topical fit to either of the programs was unclear, be it externally (to the PI) or internally (to a program director).

The next step is to look for commonalities in such scientific topics, to guide us in the process of redefining the programs.

Armed with these data, we will revisit the program descriptions, including those of other NSF entities such as the Catalysis and Biocatalysis Program in the Engineering Directorate. We will then decide if a revision of the program descriptions will suffice to clarify the distinction, or whether the SYN and CAT programs should be restructured, necessitating further community input.

Update April 2014

The first step (data mining) has been completed. A third party randomly selected 74 proposals (49 declinations, 25 awards) from the SYN and CAT programs. Two program directors (not associated with either of the programs but knowledgeable in the area) were asked to assign these proposals to either program, with only the program description at hand to guide them. They were asked not to review the jackets, so that they had no knowledge of the program that ultimately reviewed these proposals. Of the 74 proposals, both program directors independently chose the "correct" program (the program the proposals were ultimately assigned to) for 62 proposals. Proposals that were most easily binned included those without overlap between the sub-disciplines, e.g., fluorination chemistries, ligand synthesis studies, surface catalysis, etc. For the remaining 12 proposals, the test subjects chose CAT for nine proposals, when the correct program should have been SYN, and vice versa for three proposals. These proposals generally were, not surprisingly, catalysis-based proposals used in organic synthesis methodologies. While a very limited study, it underlined the need to further intellectually define catalytic topics as related to the CAT and SYN programs.

In addition to the binning experiment, in FY 2014, the SYN and CAT Programs conducted a joint CAREER panel containing proposals from both programs that were focused on catalysis-based synthetic methods. There were 8 CAT proposals and 17 SYN proposals in the panel. The reviewers had not been told prior to the panel that this was a mixed program panel, and at no point did the panelists question why a particular proposal was included in this particular panel. Each program had three proposals in the top six most highly recommended proposals. Overall, we were pleased with the results in terms of giving a very fair review to proposals on the SYN/CAT margin, but this activity did not help us to distinguish the programs.

In receiving regular IIA proposals during the September 2013 window, the Program Leads of both SYN and CAT worked diligently to separate proposals focused specifically on synthesizing new catalysts, and examining new catalytic reactivity and mechanisms from the regular SYN portfolio. Twenty-one proposals were transferred from SYN to the CAT Program and have been subsequently reviewed there. All of the affected PIs were notified of the transfer of their proposal. Some questioned the change but it was largely determined that these PIs either already had funding from the other program, or that the PIs were accustomed to working with a certain program director. Note that none of the reviewers questioned topical fit of the proposals to the program.

Finally, the SYN Program Directors examined their portfolio after the exclusion of catalysis-focused proposals. We are aware that the remaining (i.e., non-catalytic) portfolio is intellectually highly diverse - the topics span natural products synthesis to small cluster chemistries. The SYN Program will hold a special workshop in July 2014 to

encourage mid-career PIs to develop more high risk and transformational ideas related to non-catalytic synthesis. The workshop will examine needs for new reagents and improved synthetic methodologies in some of the most important industrial sectors. Results of this workshop will be publicized in a special symposium at the ACS National Meeting in Fall 2014 (San Francisco). It is hoped that this workshop will help the Program define its boundaries but also to expand into new frontier areas.

Based on these findings, the SYN program description was modified to exclude any reference to catalysis. The text that has been removed is shown as strike-through below.

"The Chemical Synthesis program focuses on the development of new, efficient synthetic methodologies and on the synthesis of complex and/or challenging molecules. Typical synthetic targets involve novel structures, structures displaying unique properties, or structures providing pathways to discover and elucidate new phenomena. Examples of supported research areas include the development of innovative reagents, ~~catalysts for synthetic transformations~~, discovery of new synthetic methods, target-oriented synthesis, green synthesis, and synthesis of novel organic, organometallic, and inorganic structures. Research in this program will generate fundamental knowledge of chemical synthesis that enables the development of new avenues of basic chemical research and transformative technologies.

Submissions that address national needs for sustainability are encouraged. Examples include the development of new synthetic methods using earth abundant and inexpensive chemicals, fundamental studies that improve our understanding of rare earth elements, and the conversion of non-petroleum based resources into useful building blocks.

The Chemical Synthesis program does not support projects whose main objectives are to study the properties of target systems even though they may contain a large synthetic component. Synthesis of nano structures, supramolecular assemblies, and polymers should be directed to the Macromolecular, Supramolecular and Nanochemistry program. Proposals containing a synthesis component but having a major focus on the mechanistic study of catalytic reactions should be submitted to the Chemical Catalysis program."

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

The report states “The present schedule, which has proposals submitted during the months of September and October, can cause problems for academic departments, many of which start their academic years in late August or early September.”

The move to one submission window was driven by the fact that although we previously had two *submission* windows, we effectively had only one *decision* window, due to misalignment with the realities of the federal budget process. Our choice of submission dates was partially guided by aligning our window with those of other Divisions, which facilitates co-review. For example, the Division of Materials Research (DMR; one of our regular partners in co-review) has a submission window that spans the months September/October, and we scheduled the window for our MSN (Macromolecular, Supramolecular and Nanochemistry) program for October, in order to best align with DMR’s window.

At this time, we feel it is unwise to change the window, as we had a significant change in the last fiscal year (i.e., a move from two to one submission windows) and we fear that a second adjustment will create confusion in the community. We will continue to collect feedback from the community and reassess this issue in fiscal year 2014.

Update April 2014
We have received no further feedback from the community on the timing of the submission window. However, through the MPS AC, the Directorate is collecting advice on review processes as a whole and may consider implementing changes to the submission/review process on a pilot basis.

"Recommendation #6: Commission a National Academies review/study of the Re-alignment of the Chemistry Division. *The composition of the review should represent a broad cross-section of the chemistry community (i.e. industry, government laboratories, and universities). The COV has provided specific scope questions to guide the assessment."*

We appreciate the thorough discussion and the many guiding questions that the Committee suggested. We further agree that a thorough assessment will include many stakeholders, including "PIs, reviewers, program officers and the broader community."

The COV felt that it was necessary to involve assessment professionals in the design of the study. The Division wholeheartedly agrees. While some of the questions can be answered by mining internal data, many of the guiding questions involve external stakeholders that would be enabled through surveys. The Division plans to address this recommendation in the coming fiscal year, with a high priority on identifying the proper entity to conduct such a study in a credible, objective, and cost-effective way.

"Recommendation #7: Work to increase more industrial partnerships. The division should consider (a) using Centers to 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. *It is important that the strength in fundamental research in the chemical sciences continue to further innovation, and the Chemistry Division can provide leadership to the community in identifying and promulgating successful industry/university collaboration mechanisms."*

We have established an internal working group that is charged with identifying stakeholders and developing a process that allows us to develop such an initiative in an informed way. Currently, NSF CHE engages with industry through GOALI (Grant Opportunities for Academic Liaison with Industry), I-Corps (Innovation Corps Teams), and our Centers for Chemical Innovation programs. In the process, we will also consider other NSF models for industry partnerships, such as those facilitated by the "Industrial Innovation and Partnerships" program in NSF's Engineering Directorate. Industrial partnerships will be an area of high priority in the coming fiscal year for CHE.

Update April 2014
The DD has met with industry stakeholders. A workshop to increase Government, Industry and Academic partnerships in the area of pre-competitive technologies is being planned for Fall 2014.

"Recommendation #8: Explore ways to increase global engagement of the chemistry community, especially faculty and students involved in projects in other countries*. CHE should seek to enhance participation in international collaborations by creating a chemical research world network of partnering agencies who share the CHE vision of a joint proposal-joint review-joint funding recommendation-parallel funding model. Exploring best practices from the Materials World Network (DMR) could provide direction on how to be effective in increasing global partnerships by the Chemistry Division."*

CHE has a very active international program ("International Collaboration in Chemistry") that has developed over the years to include a growing number of countries. It uses precisely the outlined model of collaborations between partnering agencies. The program has reached a level of maturity that allows us to re-assess the current modus operandi, with the goal of maximizing its global impact while minimizing bureaucratic burden on investigators and funding agencies.

In addition, an NSF-wide program "Science Across Virtual Institutes" or SAVI was recently launched. SAVI provides a mechanism for U.S. research communities to build long-term, structured collaborations with partnering countries in STEM fields. We expect interest in this funding mechanism to grow in the chemistry community as we continue our outreach efforts.

Update April 2014
In an effort to increase global collaboration and provide opportunities to investigators with existing collaborations, the Division issued a request to all current NSF CHE awardees, inviting them to submit supplements for international collaboration.