Report of the Committee of Visitors of the Division of Chemical Sciences, Geosciences, and Biosciences

to the

Basic Energy Sciences Advisory Committee

Review of FY 2002, 2003, and 2004

April 6-8, 2005

Germantown, MD

Executive Summary

A Committee of Visitors of the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the Office of Basic Energy Sciences reviewed nine programs in this Division on April 6-8, 2005, focusing on assessment of (1) processes used to solicit, review, and reach decisions on proposals, document decisions, and monitor progress on funded proposals; (2) how the award process has affected the breadth and depth of portfolio elements, including quality of science and the national and international standing of these elements within the boundaries of DOE missions and available funding; and (3) the programs' progress in achieving BES long-term goals. The years covered by this assessment are 2002, 2003, and 2004. Thirty-three COV members were chosen by COV Chair Gordon Brown based on expertise, and a desire to achieve a balance in terms of (1) those receiving BES support *vs.* those not receiving support; (2) members from universities, national labs and federal institutions, and industry; and (3) gender and race diversity. Each COV member was assigned to one of six subpanels representing the nine programs, with a chair from each subpanel responsible for producing a written summary of findings, comments, recommendations, and ratings of progress toward achieving long-range BES goals.

The 2005 COV found the CSGB Division to be well managed and in excellent shape, with clear evidence that the proposal solicitation, review, and action process is working well and that the quality of science, depth and breadth of portfolio elements, and national and international standing of these elements are very good to excellent in all nine programs reviewed. The number of active proposals in the Division currently numbers 931. In addition, the nine programs were rated "Excellent" in 21 categories with respect to the long-term goals of the Office of Basic Energy Sciences, with only three "Effective" ratings out of 24 applicable categories and no "Insufficient" ratings. The COV found the Division management and staff to be very responsive and well organized during the review, which greatly facilitated our assessment. The COV identified two areas requiring significant attention by CSGB Division and Office of Basic Energy Science management. One is the continuing lack of an integrated Office of Science-wide database on proposal review, tracking, decision/documentation, and monitoring (on funded proposals) processes and lack of standardized database software that allows rapid and efficient searches for information on PI's, reviewers, proposal actions, and PI productivity. The second is the need for the Office of Science to implement ways to track gender and race diversity of PI's at universities and DOE laboratories as well as the diversity of reviewers. Continuing inattention to diversity issues will have a potentially long-term adverse effect on workforce development.

We summarize below the major findings, major recommendations, and ratings of the CSGB programs.

Major Findings of the COV

1. The solicitation process for proposals is adequate for national lab scientists but requires some additional development in the case of university scientists.
2. The review process is fair, of very high quality, and very efficient in terms of time between submission and decision on renewal proposals. The time between submission and decision on new proposals should be shortened from the current one-year average. The COV found close accord between reviews and funding decisions in the proposal jackets reviewed.

3. The completeness of documentation of decisions by Program Managers was generally found to be outstanding, with only minor improvements needed in one program (*Photochemistry and Radiation Research*) in more clearly documenting the reasons for declinations.
4. The lack of an integrated Office of Science-wide or BES-wide computer database and lack of standardized database software is viewed as a major shortcoming of the proposal review, tracking, decision documentation, and funded-proposal monitoring process. This same problem was cited in the report of the 2001 CSGB COV chaired by W. Carl Lineberger, as well as in the report of the 2003 Materials Sciences and Engineering COV chaired by John C. Hemminger.
5. Monitoring of funded proposals by Program Managers is generally good and utilizes information provided in annual reports and at annual contractors meetings, as well as occasional contacts with PI's at national scientific meetings when possible.
6. Contractors meetings are viewed by the COV as extremely important to the program monitoring process by Program Managers and to individual PI's vis-à-vis their interactions with other grantees and Program Managers. Such meetings also help create research portfolios that are focused on areas relevant to the DOE mission and long-term BES goals.
7. Program Managers have too few opportunities to visit grantees at national laboratories and academic institutions or to meet with them informally at scientific conferences. The primary limitation appears to be the low travel budget available to Program Managers.
8. The quality of science funded by the CSGB programs was found to be generally outstanding, with world leading and pioneering projects in many areas and outstanding PI's in most cases.
9. There is an excellent balance of funded projects with respect to innovation, risk, and interdisciplinary research in most programs. However, the *Energy Biosciences* program is not as well integrated with other programs in the Division as it should be.
10. The COV strongly endorses the BES practice of providing long-term support to very high quality programs run by top PI's, including those in universities and national labs. We also endorse the stewardship role BES plays in providing long-term support of national lab programs and PI's, particularly for programs critical to national security.
11. Low turnover of PI's in the various programs was noted by several of the subpanels. This problem potentially could lead to slower evolution of portfolio elements than desirable with respect to new investigators and new science thrusts. An exception was noted in the *Geosciences* program where a number of new investigators have been funded over the past three years.
12. The depth of the research portfolios in the CSGB Division (as measured by total number of investigators, their career stage, the total amount of funding, and discipline diversity) is good in most cases; however, the COV found that some improvement is needed in the *Heavy Element Chemistry* program, which supports fundamental actinide and fission product research. Insufficient depth in this program may ultimately affect its viability. This program is of critical importance to the DOE mission and to our national security, and BES is the only source of funding for *Heavy Element Chemistry*.
13. Average award sizes were found to be too small for individual investigator proposals, averaging about $135K/year (NSF Chemistry averages about $150K/year for individual investigator proposals). If this average level of annual funding is continued by the CSGB Division, it could impact the retention of top PI's in the future.

14. The national and international standing of many of the portfolio elements was found to be outstanding, with unique results of high impact in many cases. One portfolio element that would benefit from careful review and evaluation is the *Radiation Research* program.
15. The integration and co-location of theory, computation, and experimentation is a unique strength of the national lab programs funded by the CSGB Division.
16. The level of diversity in BES programs in terms of career stage, race, and gender in the ranks of PI's and reviewers was thought by some COV members to be too low, although additional information is required to come to definitive conclusions as diversity data in BES are not readily available. The perceived lack of diversity in BES programs, if true, will have a potentially long-term adverse effect on workforce development.
17. The number of Program Managers in the *Energy Biosciences*, *Chemical Physics*, and *Catalysis & Chemical Transformation* programs was found to be too few and jeopardizes the future quality of these programs, given the large number of funded proposals, the complex, multi-disciplinary nature of the portfolio elements, and their importance to DOE missions and long-term BES goals.

Major Recommendations of the COV

1. The COV strongly recommends the development of standardized database software and a coherent BES-wide computer database that would include information on reviewers, proposal tracking, documentation of decisions, and funding history and productivity of investigators. The establishment of an effective database is seen by the COV as mandatory to the effective management of a program as diverse and complex as the BES research portfolio. Implementation of this recommendation would require new resources, which should be provided by the Office of Science.
2. Improved solicitation of proposals from university scientists is desirable through various avenues, including "Dear Colleague" letters of the type used by NSF and a wider distribution of program announcements. Workshop reports are generally available on the Internet (http://www.science.doe.gov/bes/chm/Publications/publications.html), and this URL should be included in all program announcements and solicitations.
3. The COV recommends inclusion of additional non-funded participants in the annual contractors meetings, particularly young investigators and underrepresented minorities, with their expenses covered by the Division when possible. This practice would enhance the impact and breadth of the program by encouraging new participants and educating both contractors and non-contractors about possible research avenues. It could also potentially address diversity issues noted earlier.
4. The annual travel budget of Program Managers should be increased by 40-50% in order to allow them to visit grantees and to attend at least two major national meetings each year, as well as one more topical conference and the annual contractors meeting. Attendance at national meetings and topical conferences should be strongly encouraged by Division (and OBES) management as part of the expected Program Manager activities.
5. In order to enhance cross-fertilization between different programs within the Division, the COV recommends that Program Managers attend contractors meetings in other Division programs when possible and potentially useful.

6. Anonymous mail reviews should be sought and used in evaluating all proposals, including multi-investigator proposals from national labs and universities, where site reviews are commonly the primary means of evaluation. This recommendation would result in an additional workload for Program Managers.
7. The BES practice of providing long-term support to very high quality research programs that address the DOE mission and long-term BES goals should be continued. The COV recognizes, however, the importance of bringing in the best new investigators when their proposed science is better than that currently being funded.
8. The COV strongly recommends that the CSGB Division consider implementing a young investigator program that would encourage younger university scientists and engineers to become involved in research relevant to the DOE mission and long-term BES goals. Implementing this recommendation would require reallocating some of the existing funding within the Division.
9. The current practice among Program Managers of setting aside funding in anticipation of renewal proposals from existing PI's limits turn-over in programs and should be carefully monitored in order to insure that the best mix of continuing and new programs is funded.
10. All programs in the CSGB Division should explore mechanisms of co-funding between programs to facilitate cross-fertilization where it makes sense. Such cross-fertilization could also be facilitated by holding joint contractors meetings when there is significant overlap between portfolio elements in different programs or when new opportunities for cross-cutting research are recognized.
11. A plan should be developed to better integrate portfolio elements in the *Energy Biosciences* program with the *Photochemistry & Radiation Research*, *Catalysis & Chemical Transformation*, and *Geosciences* programs. The COV noted a number of similar portfolio elements in these different programs as well as opportunities for significant cross-fertilization.
12. Because of the need to appoint new Program Managers in the *Energy Biosciences* program, the Division should take this opportunity to reevaluate and refocus this program in accord with the overall directions and mission priorities of BES and the Division.
13. A careful review of the organization and staffing of the *Radiation Research* program is strongly recommended as a means of increasing its national and international standing.
14. Maintain and if possible expand funding in the *Heavy Element Chemistry* program and in other areas of particular importance to the DOE mission, especially for those programs with no other realistic funding sources. This is extremely important for maintaining the workforce in areas of importance to the DOE mission.
15. In light of relatively flat funding within BES, the COV recommends that BES prioritize its funding portfolio in order to continue supporting areas critical to DOE missions at an appropriate level.
16. We recommend that the DOE should design appropriate methods to monitor gender, race, and career-stage diversity within programs through consultation with colleagues at other federal agencies. Diversity issues within the Division (and BES) could be addressed through the appointment of a Diversity Committee, which should report its findings and recommendations to the next COV. The overall goal of this effort should be to develop and nurture a diverse work force while focusing on excellent science aimed at the missions of DOE.

17. The COV recommends that the Division be allocated at least three new Program Manager positions to be distributed among the *Chemical Physics, Catalysis & Chemical Transformation*, and *Energy Biosciences* programs. These three programs are the largest in the Division in terms of number of funded proposals, and they comprise complex research portfolios in scientific areas that are evolving rapidly and hold great promise for breakthroughs in energy research.

Ratings of CSGB Programs on Progress Toward Meeting the Long-Term Goals of BES

The four long-term goals of BES can be summarized as follows: (***Goal a***) modeling, characterizing, analyzing, assembling, and using new materials and structures for energy-related applications; (***Goal b***) demonstrating progress in understanding modeling and controlling chemical reactivity and energy transfer processes in various phases, at interfaces, and on surfaces for energy-related applications; (***Goal c***) developing new concepts and improving existing methods for solar energy conversion and other major energy needs identified by BES; and (***Goal d***) demonstrating progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials. The ratings of each CSGB program with respect to progress in meeting these goals by 2015 were generally Excellent, with 21 ***Excellent*** ratings (the highest rating), only three ***Effective*** ratings, and no ***Insufficient*** ratings (the lowest rating). Four ratings of ***Not Applicable*** were assigned. See pp. 48-58 for full details.

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I. Introduction, Membership, and COV Procedures

A Committee of Visitors was convened at DOE headquarters in Germantown, MD on April 6-8, 2005, to conduct a detailed assessment of the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of BES, covering the years 2002, 2003, and 2004. The assessment focused on the following three areas, as stipulated in the charge to BESAC by Dr. Raymond Orbach, Director of the Office of Science. This charge was passed on to the COV by BESAC Chair Dr. John C. Hemminger (see *Appendix D*):

(1) Assessment of the efficacy and quality of processes used to solicit, review, recommend, and document proposal actions and to monitor active projects and programs

(2) Assessment of how the award process has affected the breadth and depth of portfolio elements and the national and international standing of these elements within boundaries of DOE missions and available funding

(3) Assessment of the program's contribution to progress in achieving BES long-term goals (see *Appendix D*, pp. 25-26 for detailed statements of these goals)

Members of the COV were selected by COV Chair Gordon E. Brown, Jr. in consultation with BESAC Chair John C. Hemminger, CSGB Director Walter J. Stevens, and members of the CSGB Division; however, Brown made the final selections. The CSGB Division consists of nine programs within three teams (Fundamental Interactions, Molecular Processes and Geosciences, and Energy Biosciences Research) that cover a broad range of scientific disciplines within the chemical sciences, geosciences, and biosciences (**Figure 1**). Because of this scientific diversity, a relatively large number of members (34) was desirable in order to provide the range of expertise needed to evaluate the large variety of research portfolios spanning these disciplines. The COV members were spread over six subpanels, including (1) *Atomic, Molecular, and Optical Science* / *Chemical Physics* (two programs), (2) *Photochemistry and Radiation Research*, (3) *Catalysis and Chemical Transformation*, (4) *Chemical Energy and Chemical Engineering* / *Separations and Analysis* / *Heavy Element Chemistry* (three programs), (5) *Energy Biosciences*, and (6) *Geosciences*. In selecting COV members, attention was paid to achieving a balance in terms of (1) members not receiving financial support from the CSGB Division (44%) *vs*. those receiving CSGB support (56%); (2) members from universities (62%), national labs and federal institutions (32%), and industry (6%); and (3) diversity of members (15% women and 3% minority). A listing of COV members and their affiliations is provided in *Appendix A* (p. 17*)*.

Prior to meetings of individual subpanels, the charge to the COV was presented by Dr. John C. Hemminger, Chair of the Basic Energy Sciences Advisory Committee. This presentation was followed by overviews of the Office of Basic Energy Sciences by Dr. Patricia Dehmer, Associate Director of Science for the Office of Basic Energy Sciences, and of the CSGB Division by Dr. Walter J. Stevens, Division Director, Dr. Eric Rolfing, Team Leader in Fundamental Interactions, and Dr. John Miller, Team Leader in Molecular Process and Geosciences. Following these overviews, COV Chair Gordon Brown discussed instructions to the COV and went over the meeting schedule. This was followed by a forty five-minute executive session of the COV, without CSGB Division staff, in which procedures were clarified and questions were answered.

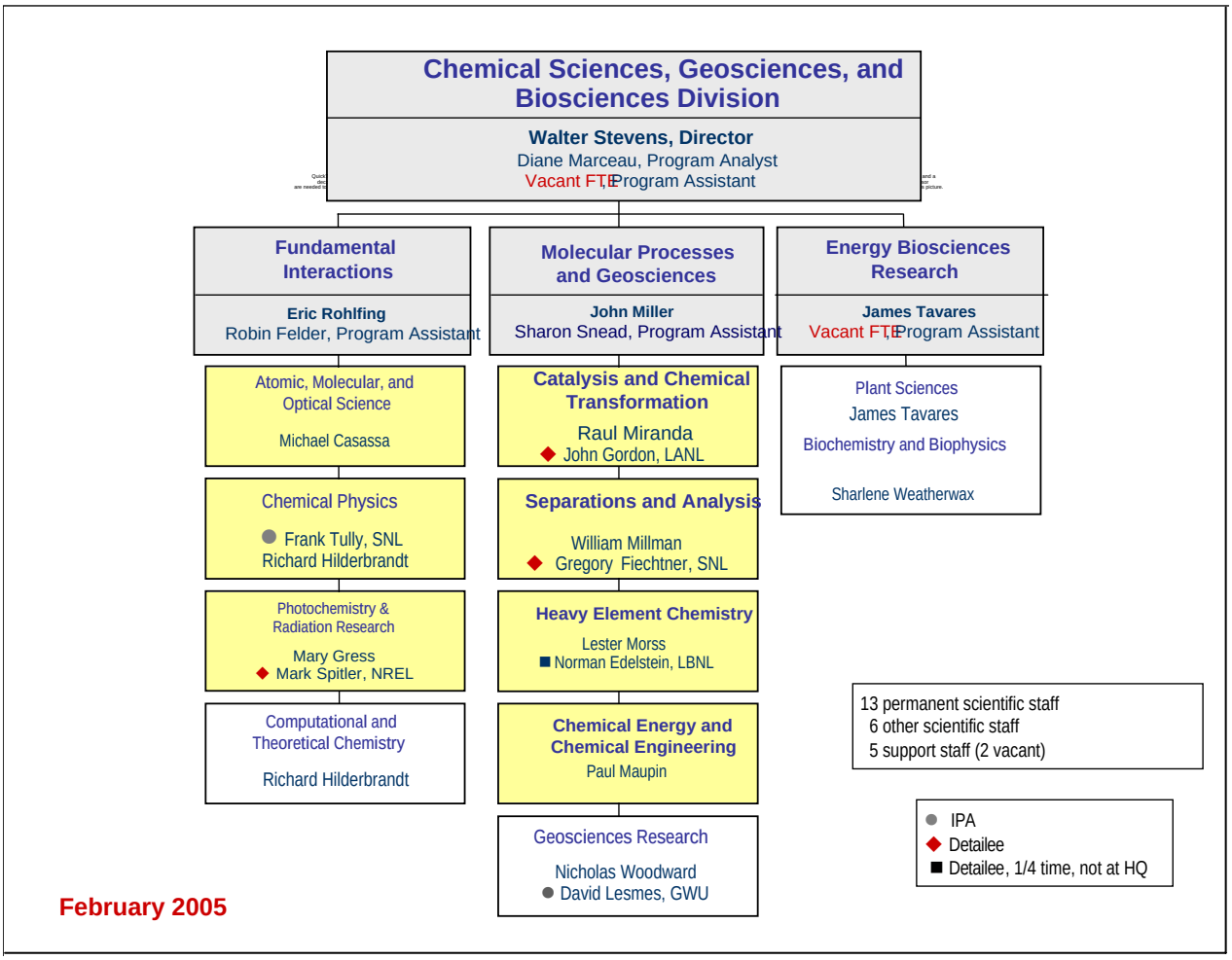


Figure 1: Organizational Chart of the Chemical Sciences, Geosciences, and Biosciences Division

The COV agenda (see *Appendix B*, pp. 18-21), which was drafted by Walt Stevens and modified by Gordon Brown, provided time for each of the six subpanels to examine about a dozen "jackets" from university and national laboratory principal investigators selected by each Program Manager as representative of their program. Several COV members felt that more time should be allocated in future COV meetings to review additional jackets. Each jacket consisted of a proposal, mail reviews, written summaries of panel reviews (for most national lab proposals and some academic proposals involving major programs), response from PI's (in some cases), correspondence between Program Directors and PI's, recommendation of the Program Manager, response of the CSGB Division Director, and summary of actions taken. Jackets from both proposals funded and proposals not funded were examined for the period 2002-2004, and all jackets within each program were available for review by each subpanel upon request. Each subpanel had a chairperson responsible for preparing a written summary of subpanel findings, comments, and recommendations, as well as ratings of programs in terms of their progress toward the goals of the Office of Basic Energy Sciences. These subpanel chairpersons also chaired a "second-read" group for each program within the CSGB Division, which followed the

"first-read" subpanel meetings. Members of the second-read group were chosen to provide a broader overview of each program and the processes used in making decisions on individual proposals. In addition, "merge meetings" were held following the first- and second-read group meetings to integrate the findings and recommendations of the primary and secondary groups of readers. Members of the first-read, second-read, and merge groups are listed in *Appendix C*.

II. Major Findings, Comments, and Recommendations of the COV

The detailed findings, comments, and recommendations of each of the six subpanels regarding assessment areas (1) and (2) above are presented in *Appendix E*. Here, we summarize the most important findings and comments, including those common to more than one subpanel. Major recommendations in response to these findings are presented in section II.B.

A. Findings and Comments

a. Solicitation of Proposals, Adequacy of Reviews and Reviewers, Decisions, Documentation

Solicitation. Most subpanels felt that the solicitation process is adequate, and that most funded proposals are consistent with the priorities and criteria stated in each program's solicitations and announcements. However, one subpanel representing three CSGB programs (*Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry*) felt that solicitations are not adequate for universities except in the case of new focused thrusts, where white papers announcing new funding opportunities are widely disseminated. In contrast, there was general consensus that solicitation of proposals from national laboratory investigators was adequate. This perceived difference may reflect the fact that national laboratories have laboratory program managers who are responsible for announcing BES proposal calls and deadlines to lab scientists and for coordinating group proposals with CSGB Division Program Managers. No such coordination exists within many universities where it is the responsibility of individual investigators to seek out BES proposal calls on the Internet or through contact with Program Managers. The fact that new investigators can submit unsolicited proposals at any time is viewed as very positive by the COV.

One subpanel (*Geosciences*) felt that it would be beneficial to clearly state in program announcements and in directions to reviewers the ongoing DOE missions and their relevance to proposal evaluation. When this point was raised by COV Chair Gordon Brown with CSGB Division management following the COV meeting, the response was that this information is not included because mission relevance evaluation is the job of the Program Managers. In spite of this response, clearer guidelines on criteria used in evaluating mission relevance would be desirable in program announcements. The *Geosciences* subpanel also felt that the common policy of discussing pre-proposals by telephone should be stated in Requests for Proposals and that RFP's should also include an up-to-date list of topical areas that are currently of interest to the program.

Review of proposals, quality of decisions, documentation of review/decision process. There was consensus among the subpanels that the proposal review process is fair and of very high quality. The reviewers chosen by Program Managers are generally adequate in number and are well

matched in expertise to the project under review, and the quality of reviews is impressive. In situations in which reviewers disagree, additional reviewers are typically enlisted by the Program Managers. The use of written assessments by proposal reviewers rather than numerical rankings (as is done by the National Science Foundation) is viewed as positive by the COV. The reviews and funding decisions were found to be in close accord for the jackets reviewed.

There was also clear evidence that the Program Managers use excellent judgment in aligning borderline funding decisions with the directions and priorities of their programs. This practice leads to research portfolios with excellent focus in most cases.

Several subpanels noted that there is a tendency to obtain a relatively high fraction of mail reviews from other program participants, which is believed to be more a reflection of low rate of review return by those not funded by the program rather than lack of effort by the Program Manager in soliciting reviews from a variety of reviewers. An inadequate number of industrial reviewers is used by Program Managers, particularly in research areas relevant to industry (*e.g.*, catalysis). No significant conflicts of interest in choice of reviewers were noted.

Another finding common to several of the subpanels is that anonymous mail reviews are not used for all proposals from national laboratories (the *Geosciences* Program is an exception as are the heavy element chemistry and catalysis programs at LANL). In those cases where only site visit teams review group proposals at national labs, anecdotal evidence suggests that this practice may lead to "softer" reviews for such proposals. Both site reviews and mail reviews serve important functions, but a number of COV members feel that it is important to avoid the appearance that review criteria are different for national labs and universities. It was also noted that national lab and university investigators are sometimes able to respond in writing to site reviewers' questions and criticisms prior to funding decisions by CSGB Program Managers. The *Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry* subpanel noted that some PI's at national laboratories do not receive critical comments from reviewers and suggested that feedback from Program Managers is sometimes lost in the chain of command at the national labs. Another finding noted by several subpanels concerned the lack of adequate documentation on "action items" resulting from the feedback provided to BES program managers at the national laboratories. As a consequence, it is difficult to determine what action national laboratory PI's had taken to correct deficiencies in proposals cited by reviewers. This shortcoming was mentioned also in the 2001 COV report. In spite of these findings, the COV applauds the ongoing efforts by CSGB Program Managers and Team Leaders to make the review process between university and national laboratory proposals more parallel, as was strongly recommended in the 2001 COV Report for this Division.

Efficiency of review process and time to decision. All of the subpanels found that the proposal submittal/review/decision process for renewal proposals was efficient in terms of time between submittal and decision, which is typically six months. When necessary, Program Managers contact reviewers to hasten responses, which helps insure a rapid decision on both solicited and unsolicited proposals. The time to decision on new proposals currently averages about one year from date of submittal, which should be reduced in order to bring it more in line with the typical 6-month decision time on new proposals at NSF. The additional time required for actions on new proposals in the CSGB Division is dependent on when they are submitted; when submitted

early in the FY, uncertainties in next FY funding slows the decision process because of the practice among Program Managers of reserving funding for anticipated renewal proposals.

Completeness of documentation in making recommendations. Documentation of the review, tracking, and decision process was found by most subpanels to be outstanding in terms of completeness. However, one subpanel (*Photochemistry & Radiation Research*) found that the reasons for declinations were not as clearly spelled out in the Program Manager's recommendations to the Division Director as is desirable, although such reasons are contained in the individual reviews. This shortcoming could result in additional work by members of the next COV in assessing documentation as well as inadequate justification for declinations in proposal action summaries prepared for Team Leaders and the Division Director.

Inadequacies of reviewer and proposal tracking database. The lack of a fully functional and integrated Office of Science-wide or BES-wide reviewer (and proposal tracking) database (and standardized database software) is seen by all subpanels as a major ongoing problem within the CSGB Division and other Divisions within the Office of Basic Energy Sciences. This problem was also noted in the 2001 Report from the CSGB COV chaired by W. Carl Lineberger and in the 2003 Report from the Materials Sciences and Engineering COV chaired by John C. Hemminger. Although a database effort does exist at the Office of Science level, it is surprisingly ineffective based on discussions with Program Managers. This shortcoming has several significant impacts on the efficient functioning of the CSGB Division, including (1) extra work by Program Managers in creating their own informal databases using spreadsheets or individually generated database software, (2) overuse of some reviewers and underuse of others, (3) inappropriate requests to former mentors or close collaborators of PI's to serve as reviewers, and (4) additional work by Program Managers in tracking the length of active grants, the number of new proposals, and portfolio turnover and in tracking the responsiveness of reviewers and quality of reviews. Although statistics on workforce diversity are not gathered by BES, if they were gathered in the future in a way similar to that used by the National Science Foundation, database software would allow the tracking of the number of women and targeted minority groups involved in BES projects and programs – a highly desirable practice.

b. Monitoring of Active Projects and Programs

Monitoring of projects and programs is accomplished by written annual progress reports, one-on-one contact between Program Managers and PI's at scientific meetings when allowed by PM travel budgets, annual contractors meetings, and, in the case of many national laboratory and multiple PI programs, site visits. The COV views the annual contractors meetings as arguably the single most important means of monitoring projects and programs and in building cohesive programs within the research portfolios of the Division. These meetings may also stimulate collaboration and synergy among laboratory and university research groups and help showcase important research findings prior to publication. Two subpanels (*Catalysis & Chemical Transformation, Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry*) noted that PI's don't always provide consistent information in the annual reports, including lack of a clear listing of publications associated with the most recent funding cycle of a proposal. They also noted that it is not clear how or if Program Managers use the material in the annual reports in monitoring projects. The main source of mid-course monitoring

of projects appears to be via the annual contractors meetings.

A major finding of the COV is that Program Managers have too few opportunities to visit grantees in both national laboratories and academic institutions, or to meet informally with them at prominent scientific conferences. This situation results from a rather low travel budget for Program Managers. Attendance at national meetings and topical conferences should be strongly encouraged as a normal part of the duties of a Program Manager.

c. Breadth, Balance, and Depth of Portfolio Elements, including Overall Quality of the Science

Overall quality of the science. All of the subpanels found that the research funded by the CSGB Division is world leading and pioneering in many areas, including

(1) coherent (quantum) control of atomic and molecular processes
(2) molecular-scale studies of heterogeneous catalysis
(3) gas phase kinetics and dynamics
(4) photochemical behavior of a variety of complex molecular assemblies, model biological materials, and liquid and membrane interfaces
(5) radiation damage in inorganic and biological materials
(6) solar energy conversion
(7) investigations of biomimetic models for photosynthesis, which could ultimately lead to direct photochemical conversion of water to hydrogen and oxygen
(8) development of noble metal nanoparticle catalysts on metal oxide supports that are highly reactive and selective
(9) mechanism-based ligand design for catalysts
(10) new catalyst design concepts from informatics-based data analysis of high through-put experiments and quantum chemistry calculations
(11) characterization of active catalytic sites and structure in complex materials using new "wet" electron spectroscopy methods at the Advanced Light Source (LBNL)
(12) heavy element and separations chemistry highly relevant to DOE missions
(13) characterization of cell wall carbohydrate components in plants
(14) development of new approaches to studies of single molecules and molecular machines
(15) studies of one carbon metabolism by bacteria, which leads to methane production
(16) studies of the photosynthetic manganese complex in plants
(17) bioengineering di-iron enzymes used for oxidation catalysts
(18) discovery and characterization of bacterial phytochromes, which has opened a new field of bacterial biochemistry
(19) use of state-of-the-art synchrotron radiation methods to probe chemical and microbial interactions at mineral-water interfaces, where most chemical reactions relevant to the Earth's near-surface environment occur
(20) development of new instrumentation for isotope ratio measurements, which has been used to understand the complicated dynamics of isotopes in nature
(21) use of molecular modeling of chemical reactions that proceed by multiple pathways in aqueous solutions
(22) use of supercomputers, which is part of the Office of Science Computing Initiative to invert three-dimensional geophysical data (see Section III, *Justification of Rating* for details).

These research areas are producing scientific results of outstanding quality by all measures considered by the COV, including scientific impact and PI recognition through awards and National Academy of Sciences memberships. These examples also illustrate the breadth and depth of the research portfolios within each of the programs of the CSGB Division.

Balance of projects with respect to innovation, risk, and interdisciplinary research. There is clear evidence that the Division has an excellent balance of projects with respect to innovation, risk, and interdisciplinary research. One example cited by the subpanel on *AMO Science* and *Chemical Physics* involved the funding of a speculative new project on development of new methods for cooling molecular beams. In spite of mixed reviews, the *AMO Science* program funded this research on a probationary basis for 18 months, after which a program review showed that the research was not meeting expectations and the funding was stopped. In spite of this lack of success, the *AMO Science and Chemical Physics* subpanel felt that this project was well worth trying and that it may eventually evolve into a technique of great use to the *AMO Science* program. Another example cited by the same subpanel is the encouragement given by BES to AMO scientists involved in planning the first experiments using the XFEL to study ultrafast atomic and molecular processes, such as the forming and breaking of chemical bonds in molecules. More generally, new initiatives, including those in nanoscience, quantum control in *AMO Science*, catalysis, and theory and computation, are having a significant impact on various CSGB programs.

Evolution of portfolios with respect to new investigators and new science thrusts. The COV found the degree of turnover in the various programs within CSGB to be low, which is related to the low number of new proposals. Although the stability of funding implicit in this low turnover rate of PI's is considered to be positive, two subpanels (*Photochemistry & Radiation Research, Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry*) felt that the current situation may ultimately limit the best mix of science being funded by CSGB. It was pointed out by the subpanel on *Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry* that only three new investigators were added to this program during the last three years. In contrast, the *Geosciences* subpanel found that a healthy number of new investigators had been added to this program during the same time period. Several of the subpanels commented that the Program Managers have worked hard to ensure evolution of portfolio elements through their active stewardship, which includes responding to community opinions about emerging research areas as expressed at contractors meetings and workshops, as well as proposal pressure.

Most of the subpanels noted that Program Managers have insufficient funding to allow them to attend a sufficient number of national meetings where they could more effectively gauge the opinions of their communities and be exposed to the most cutting edge science in a timely fashion. Increasing the number of scientific meetings attended by Program Managers could well accelerate evolution of research portfolios within CSGB programs.

The *Photochemistry & Radiation Research* subpanel noted that inclusion of non-funded participants in contractors meetings, particularly young investigators, could encourage new participants in a program and could also educate both contractors and non-contractors about possible research avenues.

Although the depth of the various research portfolios in CSGB is considered to be good by most of the subpanels, some improvement is desirable in several portfolios. One example is the *Heavy Element Chemistry* program, where insufficient depth may ultimately affect the viability of this program and further limit the number of young scientists being produced in the declining number of university groups who do heavy element chemistry. Faculty hiring practices in universities are not likely to be impacted by increased DOE funding in this mission-relevant area. Nonetheless, this particular program is considered to be of critical importance to the DOE mission, and the lack of depth could impact the viability of the future workforce in this area.

Relationship of the portfolio to other parts of the Division. The *AMO Science* program in particular couples very well with a major new initiative within BES to establish the world's first x-ray free electron laser (XFEL) – the Linac Coherent Light Source at SLAC – which is being stimulated in part by the *AMO Science* program because of the shift in emphasis from electron-atom collisions to ultrafast processes, particularly those that can be examined using 3rd and 4th generation synchrotron x-ray sources. One subpanel (*Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry*) commented on the overlap of some portfolios in various programs in BES and suggested that broader announcements of contractors meetings to grantees in different programs could further encourage cross-fertilization.

The *Energy Biosciences* program would benefit from a clearer interface with other programs in the Division such as *Photochemistry & Radiation Research*, *Catalysis & Chemical Transformation*, and *Geosciences*. For example, basic research on the mechanisms of photosynthesis and light energy conversion in microorganisms and plants could involve a combined approach of molecular, photochemical, and biophysical methods; catalytic principles as revealed from molecular studies of enzymes could lead to development of novel, useful synthetic catalysts; and synergistic research in molecular microbial geochemistry could lead to new understanding of the nanoscience of natural materials. The *Energy Biosciences* program should also capture the opportunity to include genome-enabled mechanistic research on molecular processes in microorganisms and plants in its research portfolio.

Appropriateness of award scope, size, and duration. There was a consensus among the subpanels that average award size is too low, being some $15-20K lower per year than a typical individual investigator grant from NSF-Chemistry. In light of current budget projections over the next few years, an increase in average award size could lead to fewer proposals funded. One subpanel (*Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry*) pointed out that by constraining the size of individual awards to university researchers, BES has managed to assemble an amazing range of projects aimed at DOE missions. They also pointed out that long-term funding of some of the top people in these research areas argues in favor of sustaining funding for productive scientists. However, a potential consequence of the current level of funding per PI pointed out by two subpanels (*Photochemistry & Radiation Research, Catalysis & Chemical Transformation*) is that it poses a significant risk to the maintenance of excellence the program has enjoyed, with the very best PI's potentially seeking more substantial funding for the same projects elsewhere and leaving the program. Ideally, it was felt that funding should provide support for at least two and preferably three persons (*e.g.*, two graduate students and a post-doc) per year per grant. This same subpanel expressed some concern regarding the (larger) size of grants made to individual PI's who hold

joint university and national lab appointments, relative to average award sizes to university researchers without national lab affiliations.

In light of relatively flat or declining funding for research projects within BES, the COV feels that BES must continue to prioritize its funding portfolio in order to continue supporting areas critical to DOE missions. In order to achieve this goal, it may be necessary to consider reducing the size of some portfolio elements or programs. The subpanel responsible for review of the *Heavy Element Chemistry* program felt that this program does not have access to other sources of federal funding and that this should be considered when prioritizing the mix and amount of funding among BES programs.

The COV strongly supports the BES practice of providing long-term support to very high quality programs. Such long-term stability has been very important to the success of past and current BES programs by attracting top PI's and leading to many successes in research that require sustained support of individual PI or multi-PI projects over a number of years. While turnover in programs is necessary to bring in new PI's, it should be not be done at the expense of long-term, highly successful PI's who continue to be productive and innovative and address the DOE mission. This is especially true of top national laboratory PI's whose continuing employment depends on their success in garnering DOE research funding on a continuing basis. However, renewal proposals that do not meet the scientific standards set by new proposals should not be funded. In this regard, the common practice by Program Managers of setting aside funds for anticipated renewal proposals should be carefully monitored to help ensure that the highest quality science is ultimately funded, either through renewal proposals or new proposals.

d. National and International Standing of the Portfolio Elements

Uniqueness, significance, and scientific impact of the portfolios. There was the general finding among the subpanels that the various program portfolios are having great impact, with numerous examples cited. A common comment was the importance of a close coupling of theory and experiment. *AMO Science* should be considered an enabling science because of its use of photons, electrons, neutrons, and heavy ions in research on basic physics at the quantum scale. As such, it has many connections with and significant impact on many research areas of interest to BES, including complexity, physics of extreme conditions (short time scales and high temperatures), and the use of lasers to control interactions and make new quantum structures. The *Chemical Physics Program* in gas phase kinetics and dynamics is considered to be a unique, world-leading activity relevant to combustion, and thus impacts the broader energy mission of DOE. One unique aspect of this program is that one of its major aims is to gain predictive capabilities for combustion, which is at the heart of almost all energy usage. One recent success in this program is the new understanding of combustion processes in diesel engines gained by applications of laser-induced fluorescence. Newer research activities in the *Chemical Physics* portfolio include surface physics aimed at understanding chemical reactivity on the molecular level at interfaces and in clusters. This area is also a major emphasis in the *Geosciences* program where the focus is on natural materials, including nanoparticles and interfaces.

The research portfolio in the *Photochemistry & Radiation Research* program received mixed reviews. Part of the portfolio is uniquely focused on the science of photo-initiated events

in the context of energy-related problems and includes many world-leading groups. In contrast, elements of the *Radiation Research* program are not considered as strong by the COV. The COV considers the *Catalysis & Chemical Transformation* portfolio to constitute the nation's leading program in catalysis. However, there was some concern expressed by the *Catalysis & Chemical Transformation* subpanel that care should be taken not to overemphasize multi-investigator, multi-disciplinary programs relative to single investigator programs in the more technologically driven research on catalysis. Another example of scientific impact was provided by the subpanel on *Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry* who cited the unique computer program SIMION, which is used almost universally to model ion motions in mass spectrometers and was created by scientists funded by the CSGB program. The same subpanel also pointed out that integration and co-location of theory, computation, and experimentation is a unique strength of the national lab programs. This practice has led to synergy and notable achievements in catalysis, thermophysical properties of fluid mixtures, protein structure and function, and properties of electrolytes.

Stature of portfolio principal investigators in their fields. All of the subpanels found that the PI's supported by the CSGB Division are generally excellent and include Nobel Laureates, many National Academy of Sciences members, and winners of major awards in their disciplines. In the Energy Biosciences program alone, more than 20 scientists funded by this program have been elected to the National Academy of Sciences.

Leadership position of the portfolios in the nation and world. The *AMO Science* and *Chemical Physics* portfolios lead the nation and world in gas-phase chemical kinetics and dynamics, synchrotron light source development, and VUV spectroscopy. They have also achieved national and world leadership positions in several new areas, including condensed phase and interfacial chemical dynamics, quantum control of atoms and molecules, and nanoscience. Solar energy conversion, which is the largest single component of the *Photochemistry & Radiation Research* portfolio, has also achieved very high standing. Catalysis research funded by the Program in *Catalysis & Chemical Transformation* is considered to be the best in the US. Groundbreaking work funded by *Energy Biosciences* helped lead to the recognition of a third kingdom of organisms, the *Archea*. Also noteworthy is the leadership position of the *Energy Biosciences* portfolio in research on photosynthesis in plants. In the *Geosciences*, world-leading research on interfacial geochemistry and geomicrobiology comprises a major part of the portfolio of this program.

e. Diversity Issues

Although the COV was not asked to consider diversity issues and was provided no information on diversity by the CSGB Division, the COV perceived a lack of diversity—career stage, race, and gender—in many facets of the BES program. Women, targeted minorities, and young investigators were felt to be underrepresented in the ranks of PI's, reviewers, and program managers. If our impressions are correct, this will have potentially long-term adverse effects on workforce development and on the quality of the programs in BES.

f. Staffing Issues

Three of the CSGB programs (*Chemical Physics, Catalysis & Chemical Transformation*, and *Energy Biosciences*) have larger than average proposal loads, with 166, 135, and 266 proposals currently funded, and comprise large, complex research portfolios in scientific areas that are evolving rapidly and hold great promise for breakthroughs in energy research. It was clear to the COV that effective management of each of these three programs requires more than one program manager to handle the large proposal volume and the complex, multidisciplinary nature of the portfolios.

B. Recommendations

a. Solicitation of Proposals, Adequacy of Reviews and Reviewers, Decisions, Documentation

1. In light of the demonstrated ineffectiveness of the Office of Science wide database, we strongly recommend that BES take on the task of establishing an effective database under the control of BES. Such a database should include (1) information on reviewers (to whom proposals were sent, who responded, reasons for not responding, areas of expertise, diversity of reviewers, conflicts of interest, evaluation of objectivity and quality of reviews, and timeliness of reviews), (2) proposal tracking, (3) documentation of decisions, (4) funding history of investigators, and (5) productivity of investigators, as measured through papers published and conference presentations made. The establishment of an effective database is seen by the COV as mandatory to the effective management of a program as diverse and complex as the BES research portfolio. This effort will require additional resources within BES, which should be provided by the Office of Science. In addition, the COV feels that it is important to track women and minorities in awards and declinations, as well as in the reviewer pool. This could be accomplished through the design and implementation of a new questionnaire, similar to the one used by the National Science Foundation in Fastlane, which would be completed by all scientists submitting proposals as well as by all scientists submitting reviews.

2. In order to increase the visibility of DOE funding opportunities to potential university investigators, a "Dear Colleague" letter similar to that used by NSF should be drafted and sent to all university Offices of Projects and Grants and department chairs in disciplines relevant to the CSGB Division programs.

3. It would be beneficial to articulate programmatic constraints and directions in Program Announcements and in directions to the reviewers. These criteria could include: (i) quality of the proposed science, (ii) long-term productivity and stature of the investigators, (iii) relationship of the proposal to ongoing DOE missions, (iv) use of DOE facilities, and (v) responsiveness of the proposal to long- and short-term DOE mission directives.

4. Anonymous mail reviews should be sought and used in evaluating all proposals, including multi-investigator proposals from national labs and universities, without precluding the continued use of onsite review panels. This recommendation, if implemented, would increase the workload of individual Program Managers.

5. Greater use should be made of reviewers from industry, especially in programs relevant to industrial and technological research areas.

6. We recommend documenting telephone and verbal communications between PI's, CSGB Program Managers, and national laboratory program managers, especially when problems are identified. Furthermore, there should be documentation of follow-up actions.

7. We recommend that the following information be routinely requested from PI's at the time of proposal submission: (i) a list of collaborators and others, including mentors, with a possible conflict of interest, (ii) recommendations of suggested and excluded reviewers, and (iii) information on the diversity of the PI's and co-investigators.

8. The COV sees no downside to providing verbatim reviewers' comments directly to individual national lab PI's.

9. Consistent completion of the summary logic for final funding decisions at the time of preparation of the summary document is strongly recommended for all proposals. Such a practice would improve overall efficiency and accountability.

10. We recommend inclusion of additional non-funded participants in the annual contractors meetings, particularly of young investigators. Their expenses should be covered by the program. This practice would enhance the impact of the program by encouraging new participants and educating both contractors and non-contractors about possible research avenues.

11. As the DOE moves toward center or multi-PI support, it is important to require a section in proposals on how any new or initiative-driven research relates to other funded research in order to minimize "double funding".

12. To the extent possible, plans should be developed for continuity in program management within each program so there are not single-point failure modes for vital programs (*e.g.*, sudden departure of a Program Manager).

b. Monitoring of Active Projects and Programs

1. Program Managers should have sufficient travel budgets to allow them to visit grantees occasionally at national labs and academic institutions and to attend at least two major national meetings each year as well as the annual contractors meeting and one more topical conference. Program Managers should be strongly encouraged to consider such meeting attendance as part of their normal duties. Implementing this recommendation would likely require 40-50% more travel budget than is currently available.

2. Better statistical tools would enhance the ability to monitor program portfolios. We recommend that such tools be incorporated into the database and standardized database software recommended in section II.B.a. above.

3. PI's should be required to adhere more closely to annual report guidelines.

4. Contractors meetings should be continued and, occasionally, should be held in conjunction with other scientific gatherings that will likely be attended by the grantees as well as unfunded scientists and scientists from underrepresented groups who might be invited to attend the contractors meeting. This occasional practice would reduce travel costs for participants. A possible downside to this suggestion pointed out by one COV member is the distraction factor created by holding the contractors meeting just before or just after a national meeting.

5. When possible and potentially useful, we recommend that Program Managers attend contractors meetings in other Division programs.

c. Breadth, Balance, and Depth of Portfolio Elements, including Overall Quality of the Science

1. The COV strongly endorses the BES practice of providing long-term support to very high quality research programs, and we recommend that this practice be continued when it results in the best science being funded that also addresses the DOE mission and long-term BES goals. This long-term funding stability has resulted in great successes in BES programs by attracting top PI's and producing world-class science. The COV also recognizes the importance of bringing in the best new investigators when their proposed science is better than that currently being funded. The current practice among Program Managers of setting aside funding in anticipation of renewal proposals from existing PI's limits turn-over in programs and should be carefully monitored in order to insure that the best mix of continuing and new programs is funded. An increase in the number of new proposals would help achieve this goal by providing more competition for renewals. Increased competition would also likely improve the quality of science funded by the CSGB Division.

2. We strongly recommend that the CSGB Division consider implementing a young investigator program that would encourage younger university scientists and engineers to become involved in research relevant to the DOE mission and long-term BES goals.

3. Joint contractors meetings, in which subsets of PI's from different programs are invited to attend, should be considered as a means of increasing the connections and synergism between different programs as well as the breadth of portfolio elements. The results of all contractors meetings should be made available to all CSGB Division Program Managers, if this practice is not already standard.

4. All programs within the CSGB Division should explore mechanisms of co-funding between programs to facilitate cross-fertilization where it makes sense.

5. The Division Director, in consultation with Team Leaders and Program Managers, should develop a plan to better integrate portfolio elements in the *Energy Biosciences* program with the *Photochemistry & Radiation Research*, *Catalysis & Chemical Transformation*, and *Geosciences* programs. The *Energy Biosciences* program should be maintained as an independent program within the Division.

6. With the need to appoint a new Program Manager in the *Energy Biosciences* program, the Division has an opportunity to reevaluate and refocus this program in accord with the overall directions and mission priorities of BES. Such refocusing could synergistically invigorate other programs and potentially lead to a new unique, cutting-edge research thrust for the *Energy Bioscience* program, thereby expanding its importance as a unique fundamental research program within the US federal funding landscape.

7. Metrics should be developed and monitored so that the success and impact of funded research can be evaluated by future Committees of Visitors and within the DOE. Suggested criteria for these metrics include: (i) number of published papers; (ii) citation impact and frequency; (iii) presentations at sponsored workshops and symposia; (iv) use of DOE facilities by the projects; and (v) particularly notable discoveries made as a result of funding by the program. Implementation should not be delayed and need not wait for the development of an elaborate software package; if necessary, the gathering of this information could be accomplished with in-house software using a simple database.

d. National and International Standing of the Portfolio Elements

1. Readily available computing resources (not necessarily massively parallel) should be developed to benefit all programs within BES.

2. A careful review of the organization and staffing of the *Radiation Research* program is strongly recommended as a means of increasing its national and international standing.

3. Maintain and, if possible, expand funding in *Heavy Element Chemistry* and in other areas that are important to the DOE mission and have no other realistic sources of funding.

e. Diversity Issues

1. We recommend that the DOE should design appropriate methods to monitor gender, race, and career-stage diversity within Office of Science programs through consultation with colleagues at other federal agencies. This will not be a simple task because of issues of confidentiality; however, it is important to begin this process as soon as possible. The overall goal of this effort should be to develop and nurture a diverse work force while focusing on excellent science aimed at the missions of DOE.

2. BES management should consider appointing a Diversity Committee to gather data where legally possible and practical on the level of gender, race, and career-stage diversity within the CSGB Division with respect to reviewers and PI's. This committee should also be charged with developing a plan to improve the level of diversity. A report from this committee should be made to the next COV on progress in and future plans for increasing diversity in CSGB programs. Hopefully, by the time of the next COV, recommendation e1 will have been implemented and a more general response to the need for monitoring and increasing diversity within the Office of Science will be possible.

3. Program Managers should present an overview of opportunities within BES at national meetings of underrepresented groups (*e.g.*, NOBECChE, NSBP, SACNAS) so as to target

underrepresented groups and/or during site visits to universities so as to reach out to a broader community.

4. A program that has starter grants aimed at new investigators should be designed and implemented. Such grants could be shorter in duration than regular grants. If such a program is developed, it should be highly visible, and information regarding this opportunity should be widely disseminated to the scientific community. Implementation of this new program would require new funding within the CSGB Division or reallocation of existing funding.

5. BES should initiate a program that invites Department Chairs from Historically Black Colleges and Universities to nominate a minority faculty member who has overlapping interests with the DOE mission to attend a contractors meeting. The Program Managers could meet to select 3-4 faculty members from the nominees to attend the contractors meeting at which time they can explore mechanisms for soliciting competitive proposals from this underrepresented group.

f. Staffing Issues

1. There is a serious need for additional program management staff in the CSGB Division in the three largest programs (*Chemical Physics, Catalysis & Chemical Transformation,* and *Energy Biosciences*). These programs are comprised of large, complex research portfolios in scientific areas that are evolving rapidly and hold great promise for breakthroughs in energy research. The COV recommends that the Division be allocated at least three new Program Manager positions in order to fulfill the needs of these important programs. The continued excellence of these programs will be seriously jeopardized if adequate program management staff is not assigned.

III. Ratings of Progress Toward Long-Term Goals of OBES by Program

The COV was asked to rate each of the programs reviewed with respect to their progress in meeting the long-term (by 2015) goals of the Office of Basic Energy Sciences. The four goals are as follows:

Goal a. *By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.*

Goal b. *By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.*

Goal c. *By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.*

Goal d. *By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.*

The ratings [Excellent, Effective, Insufficient, Not Applicable (N.A.)] are listed in the table below. Detailed justifications for each rating are given in *Appendix F* (pp. 48-58).

Program	Goal a	Goal b	Goal c	Goal d
AMO Science	Excellent	Excellent	Excellent	Excellent
Chemical Physics	Excellent	Excellent	N.A.	Excellent
Photochemistry & Radiation Research	Excellent	Excellent/ Effective	Excellent	N.A.
Catalysis & Chemical Transformation	Excellent	Excellent	Effective	Excellent
Chemical Energy & Chemical Engineering / Separations & Analyses / Heavy Element Chemistry	Excellent	Excellent	Excellent	Effective
Energy Biosciences	Excellent	Excellent	Excellent	N.A.
Geosciences	N.A.	Excellent	Excellent	Excellent

The ratings of each program generally fall in the "Excellent" category for most of the goals, with two "Effective" ratings, one Excellent/Effective rating, and no "Insufficient" ratings. Ratings of "Not Applicable" were given in four cases.

Appendix A: COMMITTEE OF VISITORS MEMBERSHIP

Gordon Brown - Stanford University (Chair)

Subpanel I - AMO Science / Chemical Physics (164 active proposals)
Bucksbaum, Philip - University of Michigan (Chair)
Flynn, George - Columbia University
Francisco, Joe - Purdue University
Head-Gordon, Martin - Lawrence Berkeley National Laboratory
Kay, Bruce - Pacific Northwest National Laboratory
Lucatorto, Tom – National Institute of Standards and Technology

Subpanel II - Photochemistry and Radiation Research (59 active proposals)
Rossky, Peter - University of Texas (Chair)
Ellis, Art - National Science Foundation
Fleming, Graham - Lawrence Berkeley National Laboratory
Whitten, David - QTL Biosystems

Subpanel III - Catalysis and Chemical Transformation (135 active proposals)
Bercaw, John – California Institute of Technology (Chair)
Chisholm, Malcolm - Ohio State University
Friend, Cynthia - Harvard University
Hopkins, Michael - University of Chicago
Kaldor, Andrew - Exxon-Mobil Corporation
Tumas, Bill - Los Alamos National Laboratory

Subpanel IV - Chemical Energy and Chemical Engineering / Separations and Analyses / Heavy Element Chemistry (155 active proposals)
Hieftje, Gary - Indiana University (Chair)
Chaka, Anne - National Institute of Standards and Technology
Clark, Sue - Washington State University
Murray, Royce - University of North Carolina
Sattelberger, Alfred - Los Alamos National Laboratory
Winograd, Nick - Pennsylvania State University

Subpanel V - Energy Biosciences (266 active proposals)
Richards, Jack – California Institute of Technology (Chair)
McCann, Maureen - Purdue University
Ort, Donald - University of Illinois, Urbana-Champaign
Shanklin, John - Brookhaven National Laboratory
Spormann, Alfred - Stanford University

Subpanel VI - Geosciences (152 active proposals)
Blum, Joel - University of Michigan
Casey, William - University of California, Davis
Glass, Robert - Sandia National Laboratory, Albuquerque
Nagy, Kathryn - University of Illinois, Chicago
Wallace, Terry - Los Alamos National Laboratory
Wesolowski, David - Oak Ridge National Laboratory

Appendix B: FINAL COV AGENDA

Basic Energy Sciences Advisory Committee
Committee of Visitors for the
Chemical Sciences, Geosciences, and Biosciences Division
April 6-8, 2005

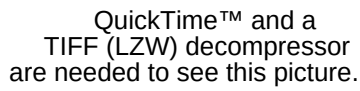
Tuesday, April 5, 2005				
Time	Activity	Committee Members	Division Staff	Location
6:30 PM	Informal Reception/Cash Bar	All	All	Marriott
Wednesday, April 6, 2005				
Time	Activity	Committee Members	Division Staff	Location
8:00 AM	Travel from Marriott to DOE Germantown	All	Drivers/Vans	Marriott Lobby
8:50 AM	Welcome and Charge to the Committee	All	John Hemminger, Chair Basic Energy Sciences Advisory Committee	A-410
9:00 AM	Welcome and Overview of Basic Energy Sciences	All	Pat Dehmer, Associate Director of Science for Basic Energy Sciences	A-410
9:30 AM	Overview of the Chemical Sciences, Geosciences, and Biosciences Division	All	Walt Stevens, Director Chemical Sciences, Geosciences, and Biosciences Division	A-410
10:00 AM	Procedures and documentation for university grants and the use of Contractors Meetings.	All	Eric Rohlfing, Team Leader, Fundamental Interactions	A-410
10:15 AM	Procedures and documentation for DOE laboratory projects	All	John Miller, Team Leader, Molecular Processes and Geosciences	A-410
10:30 AM	Instructions and schedule	All	Gordon Brown, Chair Committee of Visitors	A-410
10:45 AM	Break and disperse to Sub-Panel rooms			Coffee in E-414
11:00 AM	**First Read Sub-panel I** Atomic, Molecular, and Optical Science Chemical Physics	**Bucksbaum** Flynn Francisco Head-Gordon Kay Lucatorto	Michael Casassa Frank Tully (IPA) Dick Hilderbrandt	A-410
11:00 AM	**First Read Sub-Panel II** Photochemistry and Radiation Research	**Rossky** Ellis Fleming Lewis Whitten	Mary Gress Mark Spitler, Detailee	E-401

11:00 AM	**First Read Sub-Panel III** Catalysis and Chemical Transformation	**Bercaw** Chisholm Friend Hopkins Kaldor Tumas	Raul Miranda John Gordon (Detailee)	E-301
11:00 AM	**First Read Sub-Panel IV** Chemical Energy and Chemical Engineering Separations and Analyses Heavy Element Chemistry	**Hieftje** Chaka Clark Murray Sattelberger Winograd	Paul Maupin Bill Millman Greg Fiechtner (Detailee) Lester Morss	G426
11:00 AM	**First Read Sub-Panel V** Energy Biosciences	**Richards** McCann Ort Shanklin Spormann	Jim Tavares Sharlene Weatherwax	E114
11:00 AM	**First Read Sub-Panel VI** Geosciences	**Blum** Casey Glass Nagy Wallace Wesolowski	Nick Woodward David Lesmes (IPA)	G-207
12:30 PM	Lunch	All		E-414 and E-401
1:30 PM	**Resume First Read Sub-Panels**	Sub-Panels		Sub-Panel Rooms
4:30 PM	COV Meeting with Senior Management	All	Pat Dehmer, Walt Stevens	E-401
5:30 PM	Return to Marriott	All	Drivers/Vans	E-401
6:30 PM	Cash bar	All	All	Marriott
7:00 PM	Dinner for COV and BES Staff	All	All	Marriott

Thursday, April 7, 2005				
Time	**Activity**	**Committee Members**	**Division Staff**	**Location**
8:00 AM	Travel from Marriott to DOE Germantown	All	Drivers/Vans	Marriott Lobby
8:30 AM	Write First Read Sub-Panel Reports	Sub-Panels	none	Sub-Panel Rooms
11:15 AM	COV Executive Session Sub-panel chair reports	All	none	A-410
12:00 PM	**Lunch**	**All**		E-414/E-401
1:00 PM	**Second Read Sub-Panel I** Atomic, Molecular, and Optical Science Chemical Physics	**Bucksbaum** Friend Kaldor Chaka Wesolowski Wallace	Michael Casassa Frank Tully (IPA) Dick Hilderbrandt	A-410
1:00 PM	**Second Read Sub-Panel II** Photochemistry and Radiation Research	**Rossky** Head-Gordon Hopkins Murray Ort	Mary Gress	E-401
1:00 PM	**Second Read Sub Panel III** Catalysis and Chemical Transformation	**Bercaw** Kay McCann Nagy Sattelberger Shanklin	Raul Miranda John Gordon (Detailee)	E-301
1:00 PM	**Second Read Sub-Panel IV** Chemical Energy and Chemical Engineering Separations and Analyses Heavy Element Chemistry	**Hieftje** Casey Flynn Francisco Glass Tumas	Paul Maupin Bill Millman Greg Fiechtner (Detailee) Lester Morss	G-426

1:00 PM	**Second Read Sub-Panel V** Energy Biosciences	**Richards** Fleming Lewis Chisholm Winograd	Jim Tavares Sharlene Weatherwax	E-114
1:00 PM	**Second Read Sub-Panel VI** Geosciences	**Blum** S. Clark Lucatorto Spormann Whitten	Nick Woodward David Lesmes (IPA)	G-207
3:30 PM	Merge reports / Formulate points for report	First Read Panels + Second Read Reps	none	Sub-panel Rooms
5:30 PM	Return to Marriott	All	Drivers/Vans	E-401
7:00 PM	Working Dinner with cash bar	All	None	That's Amore Restaurant, Shady Grove Road
Friday, April 8, 2005				
Time	**Activity**	**Committee Members**	**Division Staff**	**Location**
8:00 AM	Travel from Marriott to DOE Germantown	All	Drivers/Vans	Marriott Lobby
8:30 AM	COV Executive Session	All	none	A-410
9:15 AM	Closeout Session with COV and BES Senior Management	All	Pat Dehmer, Walt Stevens	A-410
10:00 AM	Closeout Session with COV and BES Staff	All	All	A-410
10:45 AM	COV Chair meets with Sub-Panel Chairs	COV Chair Sub-Panel Chairs	none	A-410
Thank-you!				

Appendix C: FIRST-READ, SECOND-READ, AND MERGE SUBPANEL MEMBERS



Appendix D: FIRST-READ/SECOND-READ/MERGE REPORT TEMPLATE

PROGRAM: _____

BES COMMITTEE OF VISITORS (COV)
Reviewing the Chemical Sciences, Geosciences, and Biosciences Division
Fiscal Years 2002, 2003, and 2004

Charge to the COV:

I. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
(a) solicit, review, recommend, and document proposal actions and
(b) monitor active project and programs.

II. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
(a) the breadth and depth of portfolio elements, and
(b) the national and international standing of the portfolio elements.

III. Assess the program's contribution to progress in achieving the Office Basic Energy Science long term goals (shown in III, below) that are being tracked by the Office of Management and Budget (OMB).

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

Based on the COV's study of proposal actions completed within the past three fiscal years, please provide brief findings, recommendations, and comments on the following aspects of the programs's processes and management used to:

(a) Solicit, review, recommend, and document proposal actions
Consider, for example:
- consistency with priorities and criteria stated in the program's solicitations, announcements, and guidelines
- adequate number of reviewers for balanced review; use of reviewers having appropriate expertise/qualifications; use of a sufficiently broad pool of reviewers; avoidance of conflicts of interest
- efficiency/time to decision
- completeness of documentation making recommendations

Findings:

Comments:

Recommendations:

(b) Monitor active project and programs
Consider, for example
- written progress reports
- contractors meetings
- site visits
- interactions at topical, national and other meetings;

Findings:

Comments:

Recommendations:

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

Taking into account the DOE, BES, and Division missions, the available funding, and information presented about the portfolio of funded science, comment on how the award process has affected:

(a) the breadth and depth of portfolio elements
Consider, for example:
- the overall quality of the science
- the balance of projects with respect to innovation, risk, and interdisciplinary research
- the evolution of the portfolio with respect to new investigators and new science thrusts
- the relationship of the portfolio to other parts of the Division
- the appropriateness of award scope, size, and duration

Findings:

Comments:

Recommendations:

(b) the national and international standing of the portfolio elements
Consider, for example:
- the uniqueness, significance, and scientific impact of the portfolio
- the stature of the portfolio principal investigators in their fields
- the leadership position of the portfolio in the nation and the world

Findings:

Comments:

Recommendations:

III. PROGRESS TOWARD THE LONG-TERM GOALS OF THE OFFICE OF BASIC ENERGY SCIENCES

In this section the COV should evaluate the program's contribution to *progress* toward achieving the Office Basic Energy Science long-term goals (shown below) that are being tracked by the Office of Management and Budget (OMB). The BES goals are shown below. Progress toward successfully achieving the goals should be rated using the following definitions:

Excellent: the program contributes in at least one of the following ways:

a) supported research leads to important discoveries that impact the course of others' research; new knowledge and techniques, both expected and unexpected, within and across traditional disciplinary boundaries; and high-potential links across these boundaries.

b) supported research leads to important discoveries that are rapidly and readily available and feed, as appropriate, into use or projected use by the Department's technology offices, by other federal agencies, and/or by the private sector. There is evidence of substantive interactions with the Department's technology offices.

c) supported research leads to new concepts and designs for next-generation instruments and detectors for x-ray, neutron, and electron-beam scattering and for research using electric and/or magnetic fields.

Effective: the program contributes in at least one of the following ways:

a) supported research leads to a steady stream of outputs of good quality that show the potential to impact energy research.
b) supported research leads to new instruments that are world class

Insufficient: supported research could contribute to the long term goals but currently does not contribute.

Not Applicable: the goal is not applicable to the program or sub-program being reviewed.

A. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Progress rating for the program under review (select one):
__ Excellent
__ Effective
__ Insufficient
__ Not Applicable

Comments:

B. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Progress rating for the program under review (select one):
__ Excellent
__ Effective
__ Insufficient
__ Not Applicable

Comments:

C. By 2015, develop new concepts and improving existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Progress rating for the program under review (select one):
__ Excellent
__ Effective
__ Insufficient
__ Not Applicable

Comments:

D. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review (select one):
__ Excellent
__ Effective
__ Insufficient
__ Not Applicable

Comments:

Appendix E: FINDINGS, COMMENTS, AND RECOMMENDATIONS OF INDIVIDUAL SUBPANELS

The detailed findings, comments, and recommendations of each subpanel presented below were not discussed by the COV as a whole, although all COV members had the opportunity to read and comment on all of the subpanels' findings and recommendations in their review of the draft COV report. In addition, many of the findings and recommendations common to more than one subpanel were discussed in an executive session of the COV and in a presentation of our general findings to OBES and CSGB Division Management and Staff on the last morning of the COV meeting.

A. FINDINGS AND RECOMMENDATIONS OF THE AMO SCIENCE AND CHEMICAL PHYSICS SUBPANEL

A.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) The program solicitation is listed on the web, and there are many other mechanisms to get program direction information out to the research community, including reports from contractor meetings, BESAC sponsored workshops such as the Theory and Computation in Basic Energy Sciences workshop, phone calls, and program managers appearing at Gordon Conferences, APS meetings, NSBP meetings and so on.

(2) Each program is expertly reviewed. We thought there were an adequate number of reviewers, well matched in expertise to the problem under review. The consensus of both groups within the subpanel (*AMO Science* and *Chemical Physics*) was that the detail and quality of the reviews was exceptional compared to some of the other programs. The time to decision is based on a number of external factors such as the fiscal year, and the uncertain annual budgets in the Division. Renewals are handled in 4-6 months, which is appropriate. New starts often take a year or more, but this is appropriate based on the constraints.

(3) The documentation on the review and decision process was *outstanding*, and we appreciate how much work has gone into these folders. The review analysis by the Program Managers is particularly complete, and extremely well organized. The data on the current portfolio in AMOS was particularly valuable. We think this is partly responsible for the high degree of coherence in this program.

Comments:

(1) Proposal solicitation: The current system of formal posting and informal reviewing of white papers is working well, and this is evidenced by the breadth and quality of the submitted proposals. A good number of new proposals are funded each year. New investigators can submit unsolicited proposals at any time, and these programs have seen a good influx of new people over the period of this review. It often takes up to a year to review these, mostly because of the constraints of the annual budget cycle.

(2) Reviewers: We were impressed with the quality of the reviews. In *Chemical Physics*, there are detailed records on reviewers' expertise and records on whether past reviews were useful. This provides a good "corporate memory" for the program managers. *AMO Science* cannot use this data set for the most part because the *AMO Science* community is largely distinct from *Chemical Physics*. The folders themselves are one source of reviewers. IMSC does tell which reviewers have been used in the past, but the system has very limited ability to keep the kind of statistics needed by the program managers. New reviewers, averaging about one per proposal, are added by the program managers. One reviewer usually comes from a past renewal, to provide some continuity. At least half are from outside the program. Some reviewers come from outside the US, and there is always a combination of theory and experiment on every proposal. Additionally, there is a good balance between laboratory scientists and university faculty in the reviewer pool.

(3) Generally speaking, tracking and monitoring of the course of a proposal is exemplary. These are beautiful files, complete, with good and appropriate choice of reviewers. Active stewardship is apparent in aligning borderline funding decision with the directions and priorities of the program. This could serve as a model for other programs.

Recommendations:

(1) A coherent data base for reviewers would help the whole program., and assist program officers. In addition, we feel that it is important to track women and minorities in the awards and declinations, as well as in the reviewer pool. Industrial scientists could be used more in the reviewer pool, and invited to attend contractor meetings. This is already done in Combustion Kinetics, and should be considered by other program areas.

(2) We recommend that the other programs emulate the high quality of the review and decision analyses and documentation of the *AMO Science* and *Chemical Physics* programs.

(3) The travel restrictions on Program Managers are reducing the visibility of the program to the community and inhibiting Program Manager's awareness of the field. They should have the resource flexibility to attend important meetings.

(4) The reviewers, particularly in *Chemical Physics*, should include some industrial reviewers.

(5) Diversity issues should be addressed wherever possible through improved communication with diverse communities. Some mechanism must be found to increase this contact. Workshop reports sent to minority institutions or organizations along with an invitation to attend a contractors meeting could be excellent tools to expand contact.

(b) Monitor active projects and programs

Findings:

(1) Written annual progress reports are disseminated through the contractors meetings and are also distributed in book form to potential new investigators who inquire about the program. They are readable and provide good summary snapshots of progress in the programs.

(2) Topical contractors meetings are held annually, and have many benefits for the programs. They provide coherence, promote synergy, and are helpful for both the PI's and program managers.

(3) Site visit reviews are held regularly for lab and multiple PI programs, particularly tied to renewals. We found the reports of these reviews to be quite thorough. Furthermore, one-on-

one contact between the reviewers and the investigators is always part of the process, and a major part of the reports. Mail reviews were not always conducted for laboratory reviews.

Comments:

(1) We found that the one-on-one contact is an effective and efficient way to review the program and the investigators. See the recommendations on the use of mail-in reviews.

(2) Written progress reports disseminated through contractors meetings are an outstanding way to communicate within the program, and allow program officers to manage the program more effectively.

(3) The contractors meetings are perhaps the single most important element in building a truly cohesive program. One sees time and again in these proposals and reviews the true depth of interest and real knowledge by scientists of their colleagues' research programs, because of familiarity that comes from these annual meetings. Furthermore, the meetings have been avenues for collaboration and synergy between both laboratory and university groups.

(4) The written progress reports, which are also compiled into a book for the contractors meetings, are also an excellent way to gain a snapshot of the program, and the circulation of these reports to the members of the program is very helpful.

Recommendation:

(1) While we don't perceive a current problem with fairness, we are concerned about the uneven use of mail-in reviews for laboratory programs vs. university programs. They should be considered for all programs, and should supplement site reviews for laboratory and group programs. In lab proposals, mail-in reviews can be used for parts of the program to prevent an undue burden on the reviewers.

A.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

(1) The quality of the research is world leading in several areas. New initiatives (*e.g.*, coherent control, nanoscale heterogeneous reactivity, and theory and computation) are having a significant impact already and lead research in the US in these areas.

(2) There is active stewardship by the Program Managers to evolve the programs into new important areas.

(3) The portfolio is well coordinated with other areas of the program, particularly light source development, catalysis, and theory and computation. In some cases (*e.g.*, instrument development for light sources), the *AMO Science* and *Chemical Physics* programs are critical components of a larger scientific development effort.

(4) The award size and number is managed carefully by the Program Managers to maximize the scientific impact. Looking at both the *AMO Science* and the *Chemical Physics* programs together, there is balance between new starts and continuing programs.

Comments:

(1) Expanded award size would accelerate new areas into world leading positions.

(2) In both the *AMO Science* and *Chemical Physics* programs, we found consistent efforts on the part of the Program Managers to strengthen their portfolio though the solicitation and review process.

(3) All funding decisions in the University Grants program, including the borderline ones, were carefully justified with respect to the needs and goals of the programs, and were not based solely on the probability for success.

(4) The *AMO Science* program has been moving away from emphasis on electron-atom collisions, to concentrate more on ultrafast and x-ray science. This is a clear response to the increased interest in these areas in BES, particularly for the development and utilization of third-and fourth generation x-ray light sources. They have encouraged their university and laboratory programs to think about how they might best contribute to this transition, and the results are evident in the files we examined on the COV. For example, the JRML group has transformed itself from a laboratory concentrating on collision physics, to an ultrafast and high field physics lab. This was accomplished through retirement, new hires, and also a shift in the research of some of the most active and accomplished scientists at KSU, including the present Lab Director. The proposal process has been brought to bear on this, in an attempt to guide the process and make sure that the new JRML is a world-class facility.

(5) Another example is the attempt to use flexible funding to allow researchers to attempt high risk experiments in areas that could have high benefit of real interest to the program. For example, Fink at the University of Texas proposed a speculative new method for cooling molecular beams. Reviews were mixed because the scheme was new and risky, but the potential benefits were so high that the program was given probationary initial funding of 18 months. Following that, the program was reviewed again and received a very poor showing, so that it was dropped. Nonetheless, we feel that this was a good thing to try, and that initial funding may yet pay off in having started an activity that may eventually evolve into a technique of great use to the program.

(6) One sees this healthy attempt to guide the program also in the laboratories. Methods that combine x-rays with ultrafast lasers are critical for successful research programs at future x-ray free electron lasers, so when groups decide to invest in these new areas, they are given lots of encouragement, even in the face of criticism or skepticism from reviewers. This is particularly true for the laboratory programs. The program officers clearly have a lot of respect for the review process, and sometimes permit responses and rebuttal rounds in order to smooth out these issues. Ultimately, bad reviews must be responded to, either by accepting their conclusions or modifying the program.

(7) Sometimes there are very close connections between the lab and university programs. This is particularly true when both use synchrotron light sources or other lab-based facilities. One sees here the benefit of the annual contractors meetings, through which the national lab and university components of the program meet and become familiar with each others' programs, and in some cases have initiated collaborations to their mutual benefit.

Recommendation:

(1) We recommend that the CSGB Division consider implementing a young investigator program to encourage younger university people to become involved in this critical field. For example, this could be a long-term solution to a present manpower and continuity of knowledge problems in areas such as gas kinetics and heavy element chemistry. It could also reverse the perceived secular trend in reduced number of new proposals, particularly in an

era of flat budgets. Ultimately, inadequate funding will ensure erosion of our present high standing in areas of critical importance to BES, such as light source development and new energy science.

(b) the national and international standing of the portfolio elements

Findings:

(1) The programs have evolved very significantly in order to take advantage of new opportunities in energy science. Examples include coherent control and ultrafast x-rays. Very recent new activity has occurred in chemical dynamics of heterogeneous interfacial and condensed phase systems and the burgeoning area of nanoscience. A key to the success of all these programs is the close coupling of theory and experiment.

(2) Principal investigators have appropriately high stature, and there is a good mix of younger people as well. There are Nobel Laureates, many National Academy of Sciences members, and winners of major awards in *Chemical Physics* and *AMO Science*. The CSGB Division should take pride in its sizable contributions to research as evidenced by this recognition.

(3) The portfolio leads in the following areas: gas phase chemical kinetics and dynamics, light source development, VUV spectroscopy. Several newer areas have already established world leadership positions, or are on a fast track to do so. These include condensed phase and interfacial chemical dynamics, quantum control, and nanoscience. All of these areas blend both experiment and theory and modeling.

Comments:

(1) Scientific impact. The *AMO Science* program utilizes photons, electrons, neutrons, and heavy ions for research on basic energy physics at the quantum scale. This is enabling science, so it has broad connections to many different areas of great interest to BES. Current important topics include complexity, physics of extreme conditions like short time scales and high temperatures. A new and important theme is to use lasers to control interactions and make new quantum structures, as well as learn about them.

(2) The gas phase kinetics and dynamics program in *Chemical Physics* is a unique world leading activity relevant to combustion. This is clearly relevant to the broader mission of the DOE, since almost all of energy usage originates in combustion. As a longstanding mission-related scientific program, it has achieved world dominance. It is the only research program in the US that aims to gain predictive capabilities for combustion.

(3) Newer *Chemical Physics* portfolio elements in surface physics are aimed at understanding reactivity on the molecular level, at interfaces and in clusters. This has close connections to the quantum control physics activities recently initiated in the *AMO Science* program.

(4) Part of the impact is between basic research in combustion, and technological development. The CRF is a good example of a connection between co-located basic and applied research activities. There has been some success here, for example, in understanding the combustion processes in diesel engines via techniques like laser-induced fluorescence.

Recommendation:

(1) Computing resources geared toward chemical physics (not necessarily massively parallel.) should be developed to realize the potential and maintain the leadership of this program.

B. FINDINGS AND RECOMMENDATIONS OF THE PHOTOCHEMISTRY AND RADIATION RESEARCH PROGRAM SUBPANEL

B.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) The subpanel found the processes were very effective and were generally executed in full accord with expectations. The general challenge of assigning reviews to the most appropriate and knowledgeable individuals that results directly from the lack of an integrated and fully functional reviewer database was noted by the subpanel as a continuing problem. It is very disappointing that this has not been addressed more than three years after the problem was noted by the 2001 COV.

(2) There seemed to be some tendency to obtain a relatively high fraction of mail reviews from other program participants, but it appeared to be a result of a low return rate of requested reviews from those not funded in the program, rather than from a lack of effort by the Program Manager.

(3) It was found that decision summaries produced by the Program Manager did not always spell out in summary form the actual rationale for declinations, although it could be discerned from a reading of the reviews. Thus a new reader cannot always rapidly discern the essential elements associated with each decision.

Comments:

(1) Mail reviews are not now routinely used in the case of national laboratory site visit reviews. Anecdotal evidence suggests that this can tend to soften the critique, a result that could easily be attributed to the (identifiable) site visit team.

(2) The option of grant periods beyond three years appears not to be exercised, and the reason may be additional bureaucratic barriers associated with the completion of such unusual awards.

Recommendations:

(1) A reviewer database is critically necessary to improve both the effectiveness of the review process and the efficiency of the DOE staff.

(2) The solicitation of selected (anonymous) mail reviews, in specified sub-areas of the proposal, should be instituted as a routine practice in the execution of national laboratory site visits.

(3) Consistent completion of the summary logic for final funding decisions at the time of preparation of the summary document can improve overall efficiency and accountability.

(b) Monitor active projects and programs

Finding:

(1) The Program monitors active programs rigorously. Contractors meetings are an important component of this effort. Easily discerning such characteristics as the length of active grants, the number of new proposals, and the portfolio turnover is difficult, in large part due to the

inadequacies of tracking software. Such statistics generated in a uniform way would be useful in comparing programs and in evaluating trends in this and other programs.

Recommendations:

(1) Better statistical tools would enhance the ability to monitor the program.

(2) Inclusion of additional non-funded participants in the contractors meetings, particularly of young investigators, could enhance the impact of the program by encouraging new participants and educating both contractors and non-contractors of possible research avenues.

B.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

(1) The overall quality of the science in the program is excellent. This statement is evidenced in the *Photochemistry and Radiation Research* program by specific examples of new results in material structures, fundamental science of energy and charge transfer, and new observations of chemical and biochemical behavior.

(2) While the program includes an appropriately diverse portfolio, the turnover in this program is apparently low. The number of new proposals seems quite low, as well. While the stability of funding implicit in this status can encourage risk-taking, it was a concern of the subpanel that the number of new university investigators that were being considered for new grants might be too low to ensure that the best mix of science is being funded.

(3) There are elements of the Notre Dame Radiation Laboratory (NDRL) program that fall short of the scientific level one would desire, despite individual efforts of very high quality. At the same time, the capabilities of the instrumentation at each *Radiation Research* location are limited currently, so that none of these sites can fully carry out their ideal program.

Comment:

(1) The sole stewardship of *Radiation Research* by the DOE, and the mission needs for data and modeling capability in the area, were recognized. Nevertheless, the various efforts did not seem to be uniformly well focused, or well equipped, to address those needs as currently configured.

Recommendations:

(1) One important aspect deserves particular attention, the *Radiation Research* program. It seems that none of the three programs (Argonne National Laboratory, Brookhaven National Laboratory, NDRL) are configured to address all of the problems of mission interest to the DOE, and the resources to rectify this are not available. At the same time, the scientific stature of the NDRL group, taken as a whole, is not high. It seems that consideration of a plan that would consolidate the efforts is one route that deserves careful consideration.

(2) In addition, the low number of new grants suggested that perhaps the number of investigators discouraged by initial program contact may be too large. It would be valuable to assess whether this is true, and if so, the program should consider decreasing the amount of funding that is being informally "set aside" in advance for current investigators in the portfolio.

(3) The area of photochemistry is naturally interdisciplinary. Nevertheless, it would be desirable to have a mechanism to explicitly highlight the interdisciplinary character of programs by some formal means. Currently, connections between this program and those in, *e.g.*, *Catalysis & Chemical Transformation*, *Chemical Physics*, and *Energy Biosciences*, can only be inferred. The breadth of the programs could perhaps be substantively enhanced by joint contractor meetings of a subset of PI's from these different programs.

(b) the national and international standing of the portfolio elements

Finding:

(1) The program includes many of the world's leaders in the area. It is also uniquely focused on the science of photo-initiated events in the context of energy-related problems, and is recognized as such in the scientific community. Elements of the *Radiation Research* program are not strong.

Comment:

(1) It is a source of concern that the limited size of university grants associated with flat funding levels may be beginning to discourage participation of some of the most accomplished research efforts in the area, as these can access alternative sources which can provide larger recurring support. It was recognized that the traditional greater stability of BES grants offsets this effect to some extent.

Recommendation:

(1) A careful review of the organization and staffing of the *Radiation Research* program is strongly recommended.

C. FINDINGS AND RECOMMENDATIONS OF THE CATALYSIS AND CHEMICAL TRANSFORMATIONS SUBPANEL

C.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) Reviewers are critical to unbiased and accurate evaluation of proposals.

(2) The review process and associated documentation for actions were usually thorough and appropriate. However, there is room for improvement in review process.

(3) To his credit, the Program Manager is using an informal database.

(4) We were surprised by the paucity of reviewers from industry, given the obvious relevance of this topic.

(5) The DOE is moving toward center or multi-PI interdisciplinary programs. It was not always apparent how the work in individual PI funded programs was distinct from that in multi-PI programs.

Comment:

(1) Continuity in Program Managers is essential for effective program. This has been particular problem with CCT until about three years ago.

(2) The subpanel applauds the Program Manager for significant improvement in creating a coherent and vital program.

Recommendations:

(1) Mandate a request for a list of collaborators and others with a possible conflict of interest as part of grant submission to assist in the selection of reviewers.

(2) Mentors should be listed and not solicited for reviews.

(3) Routinely request suggested and excluded reviewers from the PI.

(4) We strongly recommend creation of a standardized database for reviewers, including: who proposals were sent to, who responded, reasons for not responding (conflict of interest, unresponsive), areas of expertise, evaluation of objectivity and quality of review, timeliness. The COV particularly calls out the inclusion of reviewers from industry.

(5) Mechanisms should be developed to assure a diverse set of reviewers. The Program Manager should further develop a database that includes **diversity**. Use of reviewers from industry in *catalysis* is highly desirable and should be more widely implemented.

(6) Develop a plan for continuity in program management so there are not single-point failure modes for vital programs (*e.g.*, sudden departure of a Program Manager).

(7) As the DOE moves toward center or multi-PI support, it is important to require a section in the proposals on how any new or initiative-driven research relates to other funded research to avoid "double funding".

(8) Consider awarding renewals for longer than three years for exceptional projects, in parallel with the policy for reduced-term renewals in less-compelling cases

(9) We recommend documenting telephone and verbal communications between PI's, Program Managers, and national lab managers, especially when problems are identified. Further, there

should be documentation of follow-up actions.

(10) The subpanel sees no downside to providing verbatim reviewers' comments to individual national lab PI's.

(11) A more formal mechanism for putting national lab scientists on notice for termination is needed.

(b) Monitor active projects and programs

Findings:

(1) The institution of regular contractors meetings has had a positive impact on the overall program. This appears to be one of the main mechanisms for the Program Manager to monitor active progress.

(2) While there is currently a well-defined format for annually reporting on progress, it was not clear how the Program Manager was using this tool (*e.g.*, there was some indication that not all PIs were fully compliant).

Recommendations:

(1) Consider holding the contractors meetings at other national meetings to conserve travel expenses?

(2) Examine the efficacy of the annual reporting process.

C.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

(1) The *CCT* program supports outstanding science.

(2) The subpanel applauds the Program Manager's efforts to evolve the portfolio elements by responding to (a) community opinions of emerging areas, (b) recommendations resulting from Contractors Meetings, summaries from Council on Chemical Sciences and BESAC workshops, (c) proposal pressure, (d) reading of literature and attending scientific meetings.

(3) The portfolio has evolved towards addressing some of the most challenging aspects of catalysis science. Of particular note is the recent Catalysis Science Initiative.

(4) Some improvements are needed to better inform and focus Program Managers on emerging new areas, needs, and opportunities.

(5) It was apparent to the subpanel that the Program Managers do not have sufficient funds for travel to even a few national conferences. More active participation at scientific meetings would be desirable to accelerate evolution of the portfolios, as well as improve proposal referee base.

(6) The subpanel is concerned with the lack of transparency as regards the administration of funding for PI's with joint national lab-university appointments. The Program Manager does not appear to be able to use all the program management tools employed for other programs. There appears to be confusion and an accompanying skepticism among the general community as regards the size of individual grants, especially for scientists with university appointments. We found it difficult to ascertain the funds provided to individual PI's from the material provided to us.

Comment:

(1) Recommendations from attendees at Contractors Meetings could be self-serving to those currently funded. CCS and BESAC workshops are initiated largely by those other than PM's.

Recommendations:

(1) Workshops should be an efficient and effective means to evolve the Program Manager's portfolio. For example, the Program Managers should have access to suggesting and organizing informal, focused workshops (*e.g.*, Council on Chemical Sciences). More extensive involvement of non-DOE funded (and non-US) participants would infuse new perspectives and allow a less conflicted set of recommendations.

(2) Mechanisms should be put in place for Program Managers to attend scientific meetings, together with more travel funds, to make the Program Managers more visible and involved in science that they manage, as well as expose them to new thrusts.

(3) A more transparent reporting should be provided the COV for each PI's funding for DOE national lab-university PI's, consistent with that for university PI's not affiliated with a DOE national lab.

(b) the national and international standing of the portfolio elements

Finding:

(1) The DOE *CCT* program is the nation's leading program in catalysis, well represented with national and international awards, ACS awards, National Academy of Sciences memberships, *etc.*

Comments:

(1) For technologically driven research aimed at bringing science to the marketplace, the desirability of multi-investigator, multi-disciplinary funding is well recognized. However, the field of chemical sciences still finds a unique place for the single investigator grant. Through the commitment of time, unfettered by negotiation and administration of a collaborative effort, can a chemist devote the single-minded concentration necessary to perceive, plan, pursue, and solve a problem of singular significance.

(2) Regarding the level of funding of single investigators, funding at the level currently offered through the DOE BES program for single investigator grants poses a significant risk to the maintenance of the excellence that the program has enjoyed. Ideally, funding should allow for the support of at least two, and preferably three persons (post-doctoral or graduate students) per year if the program is going to attract and retain the best PI's. Failure to maintain this level of support will lead to a natural attrition of the very best PI's as they could seek more substantial funding elsewhere. This could lead ultimately to a lessening of the impact of the science accomplished within BES.

D. FINDINGS AND RECOMMENDATIONS OF THE CHEMICAL ENERGY & CHEMICAL ENGINEERING / SEPARATIONS AND ANALYSIS / HEAVY ELEMENT CHEMISTRY SUBPANEL

D.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) Solicitation in general does not occur for universities, except by means of broad agency announcements.

(2) In contrast, solicitation for new focused thrusts is broadly announced and response results from both national labs and universities. It might be appropriate to craft a "Dear Colleague" letter similar to that used by NSF to make the new initiatives even more widely known. This move should be simplified by assembling an appropriate database and by using electronic communication.

(3) In some programs, booklets announcing funding opportunities have been prepared, an example being "Opportunities for Discovery: Theory and Computation in Basic Energy Sciences". In our view, such booklets are extremely useful, and serve not only to announce funding possibilities to the broader scientific community, but also to advertise the portfolio of current projects and possibly to integrate areas covered by the booklet.

(4) Reviews are ordinarily requested from top people in the field of the proposal. Both panel and mail reviews take place. However, there is still no consistently used reviewer database, so there is no assurance that reviewers are not overloaded or that alternative reviewers are not being overlooked. Also, the present database does not contain some pertinent information, such as reviewer expertise or responsiveness, or a list of potential conflicts of interest (*e.g.*, students, collaborators, mentors).

(5) The number of reviewers contacted varies from one proposal to another, as is appropriate, depending on the range of material being covered in the subject of the proposal, and the response of initial reviewers. In situations in which reviewers disagree, additional reviewers are contacted.

(6) When it proves necessary, reviewers are contacted individually by the Program Manager to hasten responses. This helps to maintain a rapid response to proposals, both solicited and unsolicited. As a result, the time to decision is among the shortest among federal funding agencies.

(7) Recommendations by Program Managers to fund or decline are based on both types of reviews (panel and mail) and are very well documented.

(8) Review of programs in the national laboratory system seems to be somewhat "softer" than those for potential PIs in academic institutions. As a result, the ratio of science quality/dollar invested appears lower. Of course, we realize that the DOE has a responsibility to maintain strong science in the national laboratory complex. However, the highest standards must be maintained. In part, we perceive the latter problem as arising from the "grab-bag" nature of some proposals from national laboratories.

(9) Program Managers rely on verbal assessments by reviewers rather than simple numerical rankings. We view this as being very positive.

(10) The files were extremely well documented for grants to national laboratories. However, beyond the BES letter to the PI's, the files were not consistently well documented in regards to "action items" in the BES letter. That is, the response from a national laboratory to reviewer comments occurred early, as is appropriate. However, we could not find follow-up contacts to determine whether or not promised changes were implemented. This shortcoming was mentioned also in the previous COV report. It is consequently difficult to determine what action Laboratory PIs had taken to correct deficiencies in proposals cited by reviewers.

Recommendations:

(1) Craft a "Dear Colleague" letter similar to that used by NSF to make new initiatives even more widely known, and to a broader community.

(2) Establish a strong reviewer and grantee database, preferable in collaboration with other federal agencies.

(3) We urge Program Managers to be more proactive in soliciting new proposals, particularly from beginning investigators and in emerging areas. In our view, Program Managers should show greater willingness to fund new investigators even at the expense of established ones.

(4) Consider preparing other DOE-BES program booklets such as the one entitled "Opportunities for Discovery: Theory and Computation in Basic Energy Sciences".

(5) When proposals from national laboratories are reviewed, it is important that each component be able to stand on its own merit. However, when several planned activities are combined into a joint effort, the weaker components are sometimes carried along by the stronger ones. We urge that each component be explicitly reviewed and evaluated to avoid diluting the quality of otherwise strong programs.

(6) We believe that anonymous mail reviews are often more objective and critical than site reviews. For that reason, we suggest that all reviews of programs, at both national laboratories and academic sites, be conducted at least in part by this means.

(b) Monitor active projects and programs

Findings:

(1) Contractors meetings, in our view, are extremely beneficial, and constitute a forum in which the latest research results can be presented and valuable feedback received. In such meetings, grantees become familiar with activities underway in other funded laboratories, and with cutting-edge work in other areas. Their own programs are therefore enhanced and new research directions and potential collaborations suggested. Such gatherings serve also as valuable vehicles for Program Managers to monitor progress by grantees. In some programs, contractor meetings were summarized in a published proceedings volume, something we applaud. In our experience, the contractors meetings have not often served as vehicles to foster collaborative research.

(2) PI's are not consistent in the information they provide and the degree to which they adhere to established reporting policies. The review committee noted a number of instances in which the cumulative publications of a contract were cited, with no indication of which resulted from the most recent funding cycle. Although this information can usually be extracted from an annual report, to do so requires extra effort on the part of the DOE Program Manager. We urge that PIs be required to adhere more closely to expected report guidelines and content.

(3) Program Managers do an excellent job of managing their projects, particularly of handling each three-year renewal. The degree to which they monitor ongoing projects on an annual basis, using the annual reporting mechanism, is less clear. At present, the main source of mid-course monitoring appears to be via the contractors meetings.
(4) There is a fair amount of overlap among portfolios in various programs within BES. It would therefore be appropriate to circulate announcements of contractors meetings to grantees in different programs, to further encourage cross-fertilization.
(5) It seems that Program Managers have too few opportunities to visit grantees in both national laboratories and academic institutions, or to meet informally with them at prominent scientific conferences. This situation results from a rather low budget for such Managers.

Comment:
(1) There is a concern that some PI's at national laboratories do not receive critical comments from reviewers. Rather, the feedback is sometimes lost in the chain of command. It is essential that they receive such feedback in order to address perceived shortcomings in their programs.

Recommendations:
(1) Require PI's to adhere more closely to expected report guidelines and content.
(2) Continue contractors meetings and perhaps expand them to all programs in DOE-BES.
(3) Establish a practice of preparing a booklet that summarizes each contractor meeting. Distribute the booklet to other Program Managers within DOE-BES.
(4) Delete establishing collaborative relationships as a goal of annual contractors meetings.
(5) Continue holding two separate contractors meetings in the *Separations and Analysis* program, with one meeting devoted to *Heavy Element Chemistry* and *Separations* and the other to *Analysis*. In our view, this breakdown is appropriate, given the size of each grantee pool. However, we suggest having a few grantees from one program participate in the other, to ensure cross-fertilization. As an alternative, the Program Manager could begin each of the gatherings with a summary of highlights from the other part of the program.
(6) Consider inviting 2-3 beginning investigators to each contractors meeting, in order to familiarize them with the BES portfolio. Their expenses should be covered by the program.
(7) Consider raising, by a factor of approximately 1.5, the travel budget for Program Managers.
(8) Contractor meetings should, when possible, be held in conjunction with other scientific gatherings that will likely be attended by the grantees. This is common practice in some of the programs we reviewed, but should be consistent among the DOE programs.
(9) It would be useful if Program Managers could attend contractors meetings in other programs.

D.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:
(1) By constraining the size of individual awards to university workers, DOE-BES has managed to assemble an amazing range of projects aimed at addressing DOE missions.
(2) The depth, however, is not as great, with the greatest emphasis being in the areas of nanoscience, novel spectrometric methods of characterization, and mass spectrometry. Less

depth is found in *Heavy Element Chemistry*, something this sub-panel would like to see changed. The continuing DOE need for scientists knowledgeable in actinide chemistry, coupled with declining interest in this discipline in chemistry departments around America, makes it particularly important to sustain funding in this area.

(3) In the face of flat or declining funding for projects, DOE-BES must continue to prioritize its funding portfolio in order to continue supporting those areas more immediately critical to DOE goals. It might be necessary, in order to achieve this goal, to consider reducing the size of some programs substantially. In particular, there are funded areas, such as those in the portfolio reviewed by this sub-panel, that do not have access to other sources of federal funding, whereas some other program areas in DOE-BES have overlap with other federal agencies with substantial resources. These issues should be taken into consideration in prioritizing the mix and amount of funding among BES programs.

Recommendations:

(1) Seek ways to bring together elements from different programs from DOE headquarters concerned with heavy element research in forums that will examine mutually beneficial directions and priorities.

(2) The overall portfolio of DOE-BES might be simpler to monitor if all programs had contractor meetings and the results of those meetings were made available to all Program Managers.

(3) Bolster the program in *Heavy Element Chemistry* in order to ensure workforce continuity in this area critical to the DOE.

(b) the national and international standing of the portfolio elements

Findings:

(1) Most of the scientists being funded by the BES program are at the very top of their peer group internationally. A number of these top people have been funded for a substantial length of time, arguing for the effectiveness of the BES practice of sustaining funding for productive workers.

(2) Research being conducted is of outstanding quality and is making highly significant contributions to the knowledge base and understanding of areas important to the DOE mission.

(3) This subpanel is concerned about the need to bring new, promising investigators into the overall mix of grantees, so this record can continue into the future. In particular, only three new investigators were brought into this program during the past three years.

(4) Many areas being funded by the programs reviewed by this subpanel have no other potential sources of federal support. It is critical for the DOE and for the nation that these programs continue to flourish. Examples of this uniqueness are clearest in the *Heavy Element Chemistry* program but others exist, including solution thermodynamics.

(5) These programs have a history of excellence, having provided unique resources for other investigators and supporting scientists who have received some of the top national and international awards. An example of one such resource is the computer program SIMION, used almost universally to model ion motion in mass spectrometers.

(6) Integration and co-location of theory, computation and experimentation is a unique strength for the lab programs and has led to synergy and notable achievements. This should be encouraged an even expanded. Examples are catalysis, thermophysical propeties of fluid mixtures, proteins, electrolytes, etc.

Recommendations:

(1) Strive to bring additional new investigators into each program.

(2) Maintain and, if possible, expand funding in *Heavy Element Chemistry* and in other areas that are important to the DOE mission and have no other realistic sources of funding.

(3) Consider extending to five years awards made to senior, established investigators. This move will make DOE-BES more attractive to them, despite the currently low level of annual funding. Of course, such a move will also make the overall program less flexible and nimble, so must be used judiciously.

(4) The above recommendations are in our perceived order of priority.

(5) We recognize that the above recommendations cannot be implemented without a re-prioritization of funding within BES.

E. FINDINGS AND RECOMMENDATIONS OF THE ENERGY BIOSCIENCES SUBPANEL

E.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) Examination of jackets from the past three years show outstanding compliance to process with reviews from experts in the field which were of consistently good quality. Up to six external reviews were obtained for each proposal. The combination of mail reviews and panel reviews was appropriate. Reviews and funding decisions were in close accord.

(2) Apparent time to notification has been reduced during the period under review, for which we commend the Program Managers. We encourage reducing the period to notification to as short a time as possible.

(3) Completeness of documentation and organization in the jackets was outstanding.

Comments:

(1) The *Energy Biosciences* subpanel was uniformly impressed by the review and decision process.

Recommendations:

(1) The process used by *Energy Biosciences* for extramural applications (*i.e*., the combination of mail and panel reviews) should be continued for this program.

(2) The *Energy Biosciences* review process could be used as a model by other programs in BES.

(3) In cases with conflicting reviews, a short summary of panel discussion is useful.

(b) Monitor active projects and programs

Findings:

(1) Progress reports and published papers and site visits were effectively and appropriately used for assessing progress of the biosciences supported programs reviewed by this subpanel.

(2) Current program managers have been highly effective in their interactions at scientific meetings within their budgetary constraints.

Comment:

(1) Program officers are viewed by subpanel members and the research community in general as highly effective.

Recommendations:

(1) The timely appointment of a Program Manager(s) with expertise in biology capable of fostering links with other BES programs should be made.

(2) Given the effectiveness of Program Managers at scientific meetings, we recommend that they be provided with sufficient resources to attend relevant meetings. This is particularly important in the recruitment of young investigators to the program.

E.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

(1) The quality of science is uniformly superb.

(2) The *Energy Biosciences* program provides early seeding of areas that have become of central importance, such as the development of *Arabidopsis* as the model plant system.

(3) *Energy Biosciences* has had great success in funding fundamental research in plants and microbes.

Recommendations:

(1) *Energy Biosciences* should explore mechanisms of co-funding between different BES programs to facilitate deeper understanding of biological processes.

(2) The *Energy Biosciences* subpanel sees tremendous opportunity for developing synergistic links between *Energy Biosciences* and other BES programs.

(3) The grants in the *Energy Biosciences* program are unrealistically small; at some point grants should be increased in size at the expense of number of grants.

(4) The dual pressures of flat funding and increasing the size of annual budgets will make it more difficult to bring early career scientists into the program, which we believe is essential for the future health of the program. We therefore recommend some fraction of the budget be set aside for young investigators.

(5) The program would benefit from a more clearly articulated programmatic theme linked to BES and DOE long-term themes.

(b) the national and international standing of the portfolio elements

Findings:

(1) The *Energy Biosciences* program is a major funding stream for fundamental research of world-class quality in the plant and microbial sciences.

(2) The *Energy Biosciences* portfolio is unique and consists of programs in large part not funded by NIH, NSF or USDA.

(3) Over the lifetime of the *Energy Biosciences* program more than 20 scientists have been funded who have subsequently been elected to the NAS.

F. FINDINGS AND RECOMMENDATIONS OF THE GEOSCIENCES SUBPANEL

F.I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

(a) Solicit, review, recommend, and document proposal actions

Findings:

(1) The *Geosciences* Program Manager has done an excellent job establishing a broad portfolio in response to research directions from within the DOE and from the broader community of geoscientists, as communicated in workshops, advisory relations with the National Academy, and joint programs with the National Science Foundation.

(2) Much of the science supported by the program is pioneering and is focused both on the long-term research issues and new high-risk technologies, many of which contribute to other programs within OBES.

(3) The caliber of the research that is supported is extraordinarily high, and the list of PI's represents a broad range of seniority. The program is commended for supporting both junior and senior researchers.

(4) The committee recognizes that the Program Manager uses a range of criteria to develop and maintain a balanced portfolio of funded projects. The Program Manager is commended for his policy of obtaining rigorous mail reviews on all university and national laboratory proposals, which adds greatly to the credibility of the review process.

(5) The view of the *second-read panel* was that the *Geosciences* Program Manager is effectively managing this overall program with a progressive vision.

(6) The overall *Geosciences* program is highly productive, very competitive, and has more young investigators than is evident in many other programs. The investments in new programs and young investigators has been made during periods of flat or declining budgets because of the leadership by the Program Manager and his willingness to insist that all investigators demonstrate high productivity. He has had to make difficult decisions to end stale, and/or less-productive projects so that new work can be started. Such difficult decisions have been made in both university and national laboratory projects. This approach can serve as a model for re-invigorating the research portfolios in other programs within BES.

Comment:

(1) The review process seems to be managed well with useful documentation, adequate number of referees, a wise choice of referees, due diligence to avoid conflicts-of-interest, and reasonable times to reach a decision (~6 months).

Recommendations:

(1) We suggest that the program build upon current efforts that have been made to make the process transparent by developing a set of criteria for evaluation of each proposal that can be communicated in a consistent manner to potential PI's and to reviewers. These criteria could also be used to explain reasons for denial of funding to unsuccessful PI's.

(2) We recognize that DOE/OBES is oriented by missions and may have greater programmatic constraints than other funding agencies, such as NSF and NIH. Nevertheless, we feel that it

would be beneficial to articulate these constraints in Program Announcements and in directions to the reviewers. These criteria could include:

(a) Quality of the proposed science;
(b) Long-term productivity and stature of the Investigators
(c) Relationship of this proposal to ongoing DOE missions
(d) Use of DOE facilities
(e) Responsiveness of the proposal to long- and short-term administrative directives.

Only some of these criteria can be fairly evaluated by the referees, but the PI's and referees should be made aware of current programmatic constraints and directions. In addition, the common policy of discussion of pre-proposals by phone should be stated on RFP's along with an up-to-date list of topical areas that are currently of interest to the program.

(b) Monitor active projects and programs

Findings:

(1) The program has annual topical contractors meetings, conducts visits to research sites, and sponsors numerous national meetings. An example is the sponsorship of six workshops on cutting edge geochemistry related to nanoscience, molecular modeling, heterogeneous kinetics, synchrotron studies, etc., each of which resulted in a *Reviews in Mineralogy and Geochemistry* volume. This series of soft-cover books published jointly by the Mineralogical Society and the Geochemical Society, has been widely adopted as a low-cost textbook series ideally suited for graduate students and young professional to quickly grasp the state-of-the-art in each topical area.

(2) The subpanel's view is that the program actively monitors funded research and stays current in the latest trends and innovations in the field.

Recommendations:

(1) We recommend that software tools be established immediately to track the funding portfolio, lists of reviewers and their reviewing history, and the funding history of the investigators.

(2) Metrics also need to be developed and monitored so that the success and impact of funded research can be evaluated by future Committees of Visitors and within the DOE. Suggested criteria for these metrics include: (i) published papers; (ii) citation impact and frequency; (iii) sponsored workshops and symposia; (iv) use of DOE facilities by the projects; and (v) particularly notable discoveries made as a result of funding by the program. Implementation should not be delayed and need not wait for the development of an elaborate software package; if necessary, it could be accomplished with in-house software using a simple database.

F.II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

(1) The OBES/*Geosciences* program has done an outstanding job of identifying high-impact and pioneering research at both universities and DOE facilities and this research well serves the mission of the DOE and the general scientific community.

(2) This program is one of the largest supporters of fundamental research in the physical sciences and it is crucial to the goals of the DOE to maintain the program strength and expertise in this geoscience research.

(3) The program is healthy and is focused both on long-term research issues and new high-risk technologies.

(4) The caliber of the research that is supported is extraordinarily high, and the list of Investigators represents a group of eminent scientists of international stature.

(5) Research supported by this program has launched entirely new trends and fields of research in the geosciences.

(6) Funding levels and durations seem appropriate.

Recommendations:

(1) This subpanel applauds the fact that new investigators at the national laboratories are funded by individual grants rather than by a block grant to the lab group. This policy could be a model for other programs as it invigorates the program with new ideas, allows young investigators to get a start in their careers and encourages individual initiative.

(2) We support the practice of limiting award amounts in order to allow a wider range of proposals to be supported. The full extent of potential collaborations and synergies with other programs within the CSGB Division should be more fully realized with encouragement from upper management.

Appendix F: SUBPANEL RATINGS OF PROGRESS TOWARD LONG-TERM BES GOALS

A. Rating of Atomic, Molecular, and Optical Sciences Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

AMO Science Program Rating (a): **Excellent**

Justification of Rating (a): The multiple quantum well nanostructure work done in this program under the nanoscale initiative (Klimov) has enormous breakthrough potential for impacting solar energy conversion. Although this is not a large activity in *AMO Science*, it is very high quality, world-leading work. The multiple ion research work (MIRF/ORNL) in *AMO Science* is also unique and critical to our development of fusion energy.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

AMO Science Program Rating (b): **Excellent**

Justification of Rating (b): The *AMO Science* program has led BES in emphasizing control science at the quantum level. The work in theory and experiment on coherent control of molecular processes is at the highest level, and is seeding additional work in other programs in the US, and at the national light source facilities. The program managers have done an excellent job in both building new research programs and redirecting existing programs towards this new focus.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

AMO Science Program Rating (c): **Excellent**

Justification of Rating (c): The core thrust of this area is the control and measurement of energy flow in matter, on the quantum scale. This fundamental knowledge is essential for making materials and understanding dynamical processes. The multicharged ion research facility is providing essential knowledge for fusion reactors. The *AMO Science* program is also demonstrating high-efficiency light energy conversion through new control of nanomaterials (Klimov).

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

AMO Science Program Rating (d): **Excellent**

Justification of Rating (d): This is one of the central activities of the *AMO Science* program. New instruments in short wavelength, ultrafast, and high intensity photon physics have been developed under this program. Beamlines at the Advanced Light Source and the Advanced Photon Source have been developed and utilized to understand new materials. Ultrafast lasers have been developed to elucidate chemical and atomic processes on femtosecond, or even attosecond, time scales. These instruments are world leading, and have accelerated progress in basic atomic and chemical dynamics in the US. The control of materials at their natural time scales, and at the quantum level, is a major goal of this program, and it leads all others in its implementation in the US.

B. Rating of Chemical Physics Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Chemical Physics Program Rating (a): **Excellent**

Justification of Rating (a): A small component of the existing program is focused on heterogeneous catalysis. This effort seeks to gain a molecular scale understanding of heterogeneous chemical reactions. Despite the fact that this research is relatively new, the quality is already excellent. Both the university and lab programs are uniformly of the highest quality, and seek to gain molecular understanding of complex heterogeneous chemical reactions. These relatively new endeavors are becoming as visible as the gas phase kinetics and dynamics studies, which have been the cornerstone of this program. A number of new programs have recently begun funding for nanoscale modeling and simulation and materials for hydrogen storage. It is too soon to evaluate those now, but they are promising initiatives.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Chemical Physics Program Rating (b): **Excellent**

Justification of Rating (b): This is the core activity of the *Chemical Physics* program, and many PI's are involved. The program has breadth, depth, and extraordinarily high quality PI's. There are two Nobel laureates, and much international visibility, NAS memberships, etc. They have

made fundamental advances in our understanding of molecular structure and kinetics in both experiment and theory.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Chemical Physics Program Rating (c): **Not Applicable**

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Chemical Physics Program Rating (d): **Excellent**

Justification of Rating (d): There has been significant development, improvement, and utilization of new instruments, both by single investigators and groups at universities and national light sources. For example, Wilson Ho has used STM to manipulate, build, and study molecules on surfaces. There are five beam line instruments at the ALS that are user facilities developed in this program. These beam lines have provided important new diagnostics for combustion and chemical dynamics.

C. Rating of Photochemistry & Radiation Research Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Photochemistry & Radiation Research Program Rating (a): **Excellent**

Justification of Rating (a): Fundamental science programs within the *Photochemistry* portfolio directly address the photochemical behavior of a diverse variety of complex molecular assemblies (including dendrimers, nanoparticle assemblies, model biological materials, biomimetic materials) and alternative environments, such as liquid and membrane interfaces. These investigations will produce the detailed understanding that is necessary to design the critical elements of energy converting materials.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Photochemistry & Radiation Research Program Rating (b): **Excellent (Photochemistry), Effective (Radiation Research)**

Justification of Rating (b): The *Radiation Research* program is well focused specifically on understanding the particular subset of chemical reactions and energy transfer processes that are associated with high energy excitations, in a detail that spans a large dynamic range in both spatial and time-scales. Such research is relevant not only to radiation damage and the associated biological issues, but provides a model for corresponding development, more generally. *Photochemistry* program elements specifically address essential issues as nanoscale confinement effects on energy transport, reactant transport and solvation, and reactivity. In addition, supported projects investigate nanoscale structural effects on electron transfer and energy transport in both synthetic and biological/biomimetic structures.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Photochemistry & Radiation Research Program Rating (c): Program Rating: **Excellent**

Justification of Rating (c): Solar energy conversion is a major component of the research focus in this program, representing the largest single focused component. The supported efforts include investigations focused on diverse components of the problem, including the development of novel nanostructures for light capture and for charge separation. Further, there are major efforts addressing the fundamental science underlying such critical technologies as practical biomimetic models for photosynthesis, and that forming the basis for progress toward the ultimate goal of direct solar photochemical conversion of water into hydrogen and oxygen.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Photochemistry & Radiation Research Program Rating (d): **Not Applicable**

Justification of Rating (d): It is the view of the subpanel that the instrument development element within this program area is not a sufficiently major component of the program to justify its consideration in evaluating the progress toward the DOE's long-term goals.

D. Rating of Catalysis & Chemical Transformation Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Catalysis & Chemical Transformation Program Rating (a): **Excellent**

Justification of Rating (a): The overlap between the programs in the catalysis area and two initiatives (NSET and Catalysis Science Initiative) is viewed as a very positive development placing the program on an excellent trajectory coupling advances in materials synthesis,

including nanoscale and nanophase materials, with innovative catalysis advances. Specific examples are (a) achievement of unusually high reactivity and selectivity for catalytic oxidation by Au nanoparticles supported on TiO_2. (b) Demonstration that self-assembled nanocages impart size and shape selection to accelerate catalytic aza-Cope rearrangements by nearly 1000 fold. (c) Direct conversion of catalytic reaction energy into electric current on nanoscale Pt on GaN and TiO_2 semiconductor devices.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Catalysis & Chemical Transformation Program Rating (b): **Excellent**

Justification of Rating (b): Catalysis science and technology is at the core of energy applications as highlighted in the recent DOE-BES Catalysis Science Initiative report. The *CCT* program is leading to fundamental and new understanding of reaction pathways, catalyst active sites and transformations that will be vital to a secure energy future. Examples include (a) mechanism-based ligand design for catalysts to control the microstructure and, thereby, the mechanical and physical properties of polyolefins; (b) new catalyst design concepts based on models developed from informatics-based data analysis of high-throughput experiments and quantum-chemistry calculations; (c) optimization of conditions for maintaining catalyst size and activity through fundamental studies of Pd particles on Al_2O_3 surfaces, which are relevant to NO_x abatement.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Catalysis & Chemical Transformation Program Rating (c): **Effective**

Justification of Rating (c): See comments for a and b above.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Catalysis & Chemical Transformation Program Rating (d): **Excellent**

Justification of Rating (d): Characterizing and probing active sites and structures in complex materials is critical to catalysis science. A number of excellent programs at universities and national laboratories are using and, indeed, driving the development of major BES facilities to address fundamental catalysis understanding. Examples are the high-pressure XPS facility at the Advanced Light Source at LBNL, the Chemistry beamline at NSLS, and the X-ray facilities at the Advanced Photon Source being used to probe catalyst structure by the Northwestern group.

E. Rating of the Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry Program Rating (a): **Excellent**

Justification of Rating (a): In particular, we point to the contributions of the *Chemical Energy & Chemical Engineering* / *Separations and Analysis / Heavy Element Chemistry* programs and to the above goals of progress. Most of the scientists being funded by these programs are at the very top of their peer group internationally. A number of these top people have been funded for a substantial length of time, arguing for the effectiveness of the BES practice of sustaining funding for productive workers. Research being conducted is of outstanding quality and is making highly significant contributions to the knowledge base and understanding of areas of importance to the DOE mission. Many areas being funded by the programs reviewed by this sub-panel have no other potential sources of federal support. It is critical for the DOE and for the nation that these programs continue to flourish. Examples of this uniqueness are clearest in the *Heavy Element Chemistry* program but others exist, including solution thermodynamics. These programs have a history of excellence, having provided unique resources for other investigators and supporting scientists who have received some of the top national and international awards. An example of one such resource is the computer program SIMION, used almost universally to model ion motion in mass spectrometers. However, at present, the number of new investigators being added to the contractor pool is undesirably small.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry Program Rating (b): **Excellent**

Justification of Rating (b): Most of the scientists being funded by the BES program are at the very top of their peer group internationally. A number of these top people have been funded for a substantial length of time, arguing for the effectiveness of the BES practice of sustaining funding for productive workers. Research being conducted is of outstanding quality and is making highly significant contribution to the knowledge base and understanding of areas of importance to the DOE mission. Work being supported under the "Separations" program is addressing the most fundamental problems of interaction among species in solution. Not only do these studies address fundamental questions in separation science, they also are invaluable in many other areas of solution chemistry.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry Program Rating (c): Program Rating: **Excellent**

Justification of Rating (c): We were uncertain as to whether "major energy research needs" is not already included in "a" and "b" above.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Chemical Energy & Chemical Engineering / Separations and Analysis / Heavy Element Chemistry Program Rating (d): **Effective**

Justification of Rating (d): This area is ranked "effective" as we perceive it as being somewhat lower in activity than in categories "a" and "c".

F. Rating of Energy Biosciences Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Energy Biosciences Program Rating (a): **Excellent**

Justification of Rating (a): Pioneering advances have been made through research funded by this program in the characterization of cell wall carbohydrate components. One example of a major advance is elucidation of the structure of boron di-diester crosslinks and their function in determining the tensile strength of *Arabidopsis* stems at the CCRC. This work relates directly to the molecular basis of the strength of plant structures (*e.g.*, plant stems), and it is important for understanding biomass. The CCRC in Georgia is a unique site for studies of this type, which are rated "excellent-a". Significant progress has also bee made in genetic dissection of carbohydrate biosynthesis and hydrolysis (*e.g.*, Somerville, Keegstra, Delmer and colleagues). This very effective program focuses on how inherent genetic characteristics of plants and microbes influence the processing of sugars and is rated "effective-a". Another area of strength in this program involves the development of new approaches to studies of single molecules and molecular machines, which are nanoscale in size and represent programmed self-assembly. This world-leading work by several groups, including a National Academy of Sciences PI, has potential applications in new nanoscale biomaterials (*e.g.*, Bustamente). Understanding these processes in nature inspires synthetic mimicry. It could also be rated excellent under heading b because of its relevance to self-assembly. A final area that was reviewed by this sub-panel was 1-C metabolism, which leads to methane production. From the very early days, energy

biosciences has supported ground-breaking work in this area which helped lead to the recognition of a third kingdom of organisms, the Archea. Based on this discovery, work in this area is rated as "excellent-a". Also, because of the importance of methane as an energy source, this work contributes to renewable resources and a secure energy future. It could also be rated excellent under heading c.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Energy Biosciences Program Rating (b): **Excellent**

Justification of Rating (b): The work on structure and function of the Mn complex in plants by Sauer and Klein groups (U.C. Berkeley) plays a central role in the splitting of water into hydrogen and oxygen during photosynthesis. Understanding how photosynthetic enzymes catalyze this process provides a basis for the design of biomimetic catalysts. This work grows out of the seminal studies of photosynthesis associated with U.C. Berkeley (*e.g.*, the Calvin cycle elucidated by Nobel Laureate Melvin Calvin). For decades, these groups have made outstanding contributions that have a world-leading influence. Therefore, we rate work in this area as "Excellent". Another area funded by the Energy Biosciences Program focuses on defining the catalytic envelop and redesign of di-iron enzymes with respect to chiral fatty acid modification (*e.g.*, Shanklin, Brookhaven National Laboratory). This work shows how one can use biotechnology to understand and bioengineering to improve important biological processes, in this case oxidation catalyzed by di-iron enzymes. We rate this work as "Excellent". Another area reviewed by the *Energy Biosciences* subpanel was on theoretical energy calculations of protein transport into plastids by Theg (U.C. Davis). We found this work to be very solid and rate it as "effective". Overall, the three areas reviewed are rated excellent overall.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Energy Biosciences Program Rating (c): **Excellent**

Justification of Rating (c): One area reviewed by this subpanel focused on comparative structure-function and biophysical studies of chlorophyll antenna proteins and complementary genetic and environmental regulation studies on these proteins (*e.g.*, Blankenship and Chory). Chlorophyll antennae collect light in photosynthesis and eventually use this energy to create carbohydrates from CO_2. They are thus central to the photochemical aspects of photosynthesis. This area informs our basic understanding of this phenomenon and has significance for future DOE technology. Thus we rate it as excellent. Another area reviewed concerned structure-function-based studies of the microbial cellulosome (*e.g.*, Wu, University of Rochester, Joy, U.C. Davis), which are showing tangible progress towards microbial bio-inspired biocatalysis. This work on carbohydrate metabolism is leading to more fundamental understanding of carbohydrate biocatalysis and biomass conversion and was rated effective. Pathway engineering of

Zymomonas for increasing the diversity of sugars available for ethanol production is the focus of another area funded by *Energy Biosciences*. Increasing the diversity of sugars available has importance in the technology of alternative fuels. Engineering metabolic pathways in *Zymomonas* also addresses this issue and provides approaches that will have wider applications in engineering metabolic pathways in other organisms. The quality of the work is on the cusp between effective and excellent. A final area reviewed by this subpanel was the discovery of bacterial phytochromes by Vierstra at the University of Wisconsin. This discovery and characterization of bacterial phytochromes has opened a new field in bacterial biochemistry. The success of this research mirrors almost exactly the definition of excellent.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Energy Biosciences Program Rating (d): **Not Applicable**

G. Rating of the Geosciences Program

a. By 2015, demonstrate progress in designing, modeling, fabricating, characterizing, analyzing, assembling, and using a variety of new materials and structures, including metals, alloys, ceramics, polymers, biomaterials and more – particularly at the nanoscale – for energy-related applications.

Geosciences Program Rating (a): **Not Applicable**

Justification of Rating (a): As written, this long-term goal does not include geomaterials. However, the Earth is a rich source of natural paradigms that provide inspiration for new materials. Catalysts, for example, include zeolite materials, zero-valent metal alloys, and oxide minerals that are doped with organo-metallic sorbates from aqueous solutions. Nature has performed an experiment in combinatorial chemistry from which research on new materials could benefit greatly. Organic and inorganic nanomaterials are ubiquitous in nature and represent a broad range of chemistries and structures. The behavior of both catalytic materials and nanomaterials is based upon their surface reactivity, which has been a general focus of the *Geoscience* Program over the past decade. Porous materials take surface reactivity into the three-dimensional realm, and the imaging of this structure in geomaterials—rocks, sediments and soils—has been pioneered in the geosciences. Synthesis of new biomaterials is often based on biologically mediated mineral formation processes. Self-assembly processes are inherent to these natural systems.

The *second-read panel* felt that BES should foster more interactions between this *Geoscience* program and other programs within BES and the Office of Science. These interactions should be designed to position BES to recognize and respond to new opportunities between programs as they arise. Possible examples might be interactions between *Geosciences* and *Energy Biosciences*, or *Geosciences* and *Heavy Element Chemistry*. In the first example, interactions between two larger programs within BES may lead to fertile ideas and new discoveries in the transformation of molecules via catalytic pathways important to nature. In the second example, the broader national laboratory foundation and management style of the *Geosciences* program

may result in significant reinvigoration of *Heavy Element Chemistry*, while also broadening support for a highly mission-critical area like *Heavy Element Chemistry*.

b. By 2015, demonstrate progress in understanding, modeling, and controlling chemical reactivity and energy transfer processes in the gas phase, in solutions, at interfaces, and on surfaces for energy-related applications, employing lessons from inorganic, organic, self-assembling, and biological systems.

Geosciences Program Rating (b): **Excellent**

Justification of Rating (b): Virtually all current and future energy sources either originate from, or have enormous impacts on Earth systems, and advances in the fundamental understanding of geological processes are essential in meeting our Nation's energy needs and the quality of the environment. Because shallow subsurface processes proceed via aqueous solutions reacting with heterogeneous minerals and in rock pores, this science is inherently an aqueous and interfacial subject. Thus, the geoscience community is in the forefront of research on aqueous chemistry and surface chemistry and this research is distinct from studies of the behavior of ideal surfaces in vacuum or in low pressures of gases.

Tremendous expertise on the development of thermodynamics and kinetics of reactions in solution, and particularly at high temperatures, high pressures and in complex mixtures, now resides in Geochemistry. A distinct difference between chemical kinetics in this program, as compared with other parts of BES/CSGB is that long-term metastability and extremely slow reaction rates are typical of geological materials, presenting unique challenges in imaging, experimentally quantifying, and computationally simulating such phenomena. Furthermore, large-scale simulations are required because the complex compositions of natural minerals and fluids inherently require use of many thousands of atoms and molecules in order to achieve statistical significance. This program has pioneered approaches for studying these complex systems.

This program provides an absolutely vital service to science by determining the fundamental properties of minerals, fluids, and amorphous phases needed to build and validate coupled reaction and transport computer codes for lifetime predictions of remediation schemes as well as the impacts of energy extraction and utilization strategies.

This expertise is essential to the mission of the DOE and is not well funded by agencies apart from the DOE. The *Geosciences* program in BES supports much of the pioneering work addressing these issues, and includes a richly diverse portfolio of excellent research conducted by the most prominent scientists in the field. The program has taken advantage of advances in analytical computational and theoretical geochemistry, and its placement within the BES/CSGB Division is ideal for the transfer of new information to and from other disciplines.

Expertise needs to be added in methods of synthesizing and characterizing nanometer-sized aqueous organic and inorganic macromolecules that can serve as models for systematizing chemical kinetic studies and for understanding particle transport. This effort would draw upon the investment of the DOE in nanoparticle science and link closely to new computer methods of

predicting reaction properties in the bulk. More aggressive attempts should be made to link with other programs within BES and to contribute the traditional *Geosciences* program strengths in aqueous chemistry, complex mixtures, and research at high temperatures and pressures.

c. By 2015, develop new concepts and improve existing methods for solar energy conversion and other major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Geosciences Program Rating (c): **Excellent**

Justification of Rating (c): Geoscience research in this program has also had major impact on current energy research needs in areas such as subsurface geochemical imaging and *in-situ* reservoir chemical alteration related to long-term carbon storage. Advances in understanding aqueous interfacial chemistry that involve complex solutions and oxide mineral surfaces have considerably affected the design of catalysts, fuel cells, and solar cells based upon semiconducting oxide solids. Most energy sources either originate within the solid Earth or have impact on Earth processes. Therefore, as the nation's energy needs evolve, the *Geosciences* program will continue to be in the forefront of creating new knowledge to meet these needs.

d. By 2015, demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Geosciences Program Rating (d): **Excellent**

Justification of Rating (d): *Geosciences* researchers have been leaders in the use and development of experimental beamlines at synchrotron facilities such as the Advanced Photon Source, the Advanced Light Source, NSLS, and SSRL. Conception and use of EXAFS and x-ray standing wave beamlines at SSRL and NSLS and the highly successful GSECARS beamlines at the Advanced Photon Source, and conception and use of scanning transmission x-ray microscopy and wet photoelectron spectroscopy at the new MES beamline (11.0.2) at the Advanced Light Source have made it possible to develop the rapidly growing field of Molecular Environmental Science. One example of this work is the use of x-ray standing waves at SSRL to probe the interaction of heavy metal pollutant ions such as lead and selenium with biofilm-coated minerals surfaces. Another example is the development at Argonne National Laboratory of 'model-independent' methods of calculating the three-dimensional distributions of atoms at mineral-fluid surfaces at sub-Angstrom resolution using x-ray standing-wave measurements. Similarly, the geoscience community exploited the development by Nier and Urey of stable-isotope systematics and measurements, and research supported in this program has continued to develop new instrumentation for isotope ratio measurements and applied these instruments to understand the complicated dynamics of isotopes in nature. Similarly, the Office of Scientific Computing Initiative has been used extensively by the geosciences community in the molecular modeling of chemical reactions that proceed by multiple pathways in aqueous solutions and in the inversion of three-dimensional geophysical data, such as are obtained through seismic, electromagnetic, or other potential-field methods.