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 2008, 2009, and 2010

April 6-8, 2011

Germantown, MD

Executive Summary

A Committee of Visitors (COV) carried out a review of the programs in the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the Office of Basic Energy Sciences (BES) covering the fiscal years 2008, 2009, and 2010. Thirty-eight participants constituted the review committee, which met in Germantown on April 6-8, 2011. The charge given to the COV by John Hemminger, Chair of the Basic Energy Sciences Advisory Committee (BESAC), was to assess (1) the efficacy and quality of the 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 the national and international standing of these elements within the boundaries of DOE missions and available funding; and (3) the progress of the programs toward the BES long-term goals that have been established through the Government Performance and Reporting Act (GRPA). The format was similar to those of previous COV reviews of programs in the Office of Science. The review excluded work performed in Energy Frontier Research Centers (EFRCs), the Fuels from Sunlight Energy Innovation Hub, the Office of Science Early Career Program, and the Office of Science Graduate Fellowship Program.

The COV judged both the science supported by BES in the CSGB Division and the management and decision-making processes reviewed in the CSGB Division to be excellent. The processes for proposal solicitation and review, for awards, and for monitoring of projects were found to be executed very well, evidencing the dedication, professionalism, and strong scientific credentials of the Program Managers and the competence of the support staff. The CSGB-supported research is characterized by a strong international reputation. The programs were rated "Excellent" in all GRPA categories by all seven panels.

The COV congratulates BES and the Office of Science on its accomplishments. This Committee appreciates the careful planning and efficient, hard work of the Division management in preparing for the review and their help and responsiveness to all requests during the review.

The COV has several major recommendations:

- Program Managers are encouraged to attend more national and international conferences and to make more visits to groups of researchers in their programs—to spread the message of BES programs, to encourage wider participation, and to keep abreast of forefront research in their fields.
- The COV recommends continued use of the procedures applied in the program to consider short preliminary statements of research ideas (white papers) and to provide rapid evaluations either encouraging researchers to submit full research proposals or consider modifying their plans.
- The COV recommends that BES provide web sites that are more accessible and encouraging than those currently available to those who might be interested in participating in the program and obtaining funding.

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I. Introduction, COV Membership, and COV Review Procedures

A Committee of Visitors (COV) participated in a review of the programs in the Chemical Sciences, Geosciences, and Biosciences (CSGB) Division of the DOE Basic Energy Sciences program, evaluating work done in fiscal years 2008, 2009, and 2010. Thirty-eight participants served as COV members in this activity, which took place in Germantown on April 6-8, 2011.

According to the charge presented to the COV (Appendix A) by the Chair of the Basic Energy Sciences Advisory Committee (BESAC), John Hemminger, the Committee considered the following components of the Division:

- Atomic, Molecular, and Optical Sciences
- Chemical Physics
- Catalysis Science
- Separations and Analyses
- Heavy Element Chemistry
- Geosciences
- Solar Photochemistry
- Photosynthetic Systems
- Physical Biosciences

The committee was not charged to consider activities such as the Energy Frontier Research Centers (EFRCs), the Fuels from Sunlight Energy Innovation Hub, the Office of Science Early Career Program, or the Office of Science Graduate Fellowship Program.

The charge presented by Dr. Hemminger was: (1) to assess the efficacy and quality of the processes used to solicit, review, and document proposal actions and monitor active projects and programs and (2) within the boundaries defined by DOE missions and available funding, to comment on how the award process has affected the breadth and depth of portfolio elements and the national and international standing of the portfolio elements. In addition to the above elements, the COV was asked by Dr. Hemminger to provide input for the evaluation of BES progress toward the Government Performance and Results Act (GPRA) long-term goals, which are stated below.

The COV members were selected for their scientific expertise by COV Chair Bruce Gates in consultation with CSGB personnel. They sought a balance of the committee membership in terms of: (a) those receiving BES support *vs.* those not receiving such support; (b) membership from universities, National Laboratories and federal institutions, and industry; and (c) gender and racial diversity. A list of the COV members is presented in Appendix B. Each COV member was assigned to one of seven panels representing the nine programs listed above (Heavy Element Chemistry and Separations and Analysis were considered by a single panel, and Photosynthetic Systems and Physical Biosciences were considered by a single panel). For each panel a Lead was selected, who was

responsible for leading his/her team to produce a written summary of findings, comments, recommendations, and ratings of progress toward achieving long-range BES goals.

The evaluation of the programs followed that of the 2008 CSGB Division COV. The COV agenda is summarized in Appendix C. The most thorough examination of the programs took place during the "First Read" of the portfolio of activities in the programs most closely related to the expertise of the participating COV panelists. Panel members in groups of five or six drafted reports in the COV Template (Appendix D), including summaries of findings, comments, and recommendations. When this read was completed, the panel leads shared their results with each other and the COV Chair. These steps were followed by meetings of combined panels (two or three panels per group as summarized in Appendices C and E), providing an opportunity for assessment of program interactions and synergies. Then "Second-Read" panels convened, consisting of groups largely different from those of the "First-Read" panels (Appendix C) and having less expertise in the programs that they were evaluating. The "Second-Read" panels provided cross-checks and ensured that issues considered to be important by "First-Read" panels were aired across the programs.

The "First-Read" panels later reconvened and considered the input of the "Second-Read" panels in drafting panel reports.

The completed templates containing the evaluative comments for each of the seven panels are presented in Appendix E (to save space, not all the wording in the templates is shown in Appendix E—the reader may refer to Appendix D for the details).

Panelists were also asked to rate the progress of each program toward the long-term BES goals, and a summary of these evaluations is included in Appendix E.

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

A. Major Findings of the COV

1. The COV finds that throughout the CSGB Division the overall quality of the science is excellent by international standards. We find overall that the science supported by the CSGB Division consistently reflects both a high degree of intellectual depth and scientific breadth. The portfolios include numerous scientists who are highly regarded and well recognized at the international level.

2. The COV judges the decision-making processes and documentation reflecting the work of the Program Managers to be excellent, demonstrating the dedication, professionalism, and experience of these individuals. Their analysis is characterized by depth, thoughtfulness, and insight into the science supported by BES.

3. The Committee commends the practice of welcoming preliminary statements of potential research projects and the use of white papers that Program Managers

evaluate rapidly. These procedures allow rapid and efficient communication with potential BES investigators, help to direct the proposals that are welcomed toward projects that are in line with the BES missions, and save time of scientists who write and review proposals.

4. The COV judges that the implementation of the information management system PAMS will bring many benefits to the operations of the Division and the impact of BES-supported research.

B. Recommendations of the COV

1. Program managers are encouraged to attend more national and international conferences in the fields of science supported by their programs and to make more visits to groups of researchers in their programs, not just those in National Laboratories. The anticipated benefits of this recommended travel and these interactions include more efficient spreading of the message of BES programs, more encouragement of participation in them, and more opportunity on the part of Program Managers to be aware of the forefront research in their fields and to keep in contact with the researchers doing it.

2. The COV recommends continued use of the procedures applied in the program to consider short preliminary statements of research ideas and plans (white papers) and to provide rapid evaluations that either encourage researchers to submit full research proposals or consider modifying their plans.

3. The COV recommends that BES provide web sites that are more accessible than those now in place to facilitate outreach to the public and to encourage those who might be interested in obtaining funding and in participating in the program.

C. Other Comments and Suggestions of the COV

Many specific comments and recommendations are stated in the detailed panel reports presented in Appendix E. Several of these comments emerged from a number of the panels and in the discussions involving the whole COV on Friday morning. They are the following:

- There is a strong consensus that the PAMS system is essential, will be very helpful, and should be developed promptly.
- A number of COV members judge that it would be a good idea to fund longer-term projects (such as four-year projects) in appropriate cases when reviews are extraordinarily positive.
- There is a consensus that the program should strive for more visibility.

- The wording of the template "Progress Toward the Long-Term Goals of the Office of Basic Energy Sciences" (Appendix D) is unfortunately lacking in clarity and should be rewritten before the next COV is convened.
- The COV appreciates that the staffing of the CSGB Division of BES has reached a level sufficient to carry out the mission, but cautions that the detailees are needed and that the Program Managers and staff have their hands full.
- The COV noted progress in response to a recommendation stated in the 2008 COV Report urging that reviews of proposals for projects at the National Laboratories be focused more on plans and less on previous accomplishments.

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

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

Goal A. *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. *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. *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. *Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.*

The ratings are listed in the table below. Detailed justifications for each rating are given in Appendix E.

Program	Goal A	Goal B	Goal C	Goal D
AMO Science	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Chemical Physics	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Solar Photochemistry	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Catalysis Science	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Heavy Element Chemistry/Separations and Analysis	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Energy Biosciences	**Excellent**	**Excellent**	**Excellent**	**Excellent**
Geosciences	**Excellent**	**Excellent**	**Excellent**	**Excellent**

Appendix A: Charge to the COV

UNIVERSITY OF CALIFORNIA, IRVINE

BERKELEY • DAVIS • IRVINE • LOS ANGELES • MERCED • RIVERSIDE • SAN DIEGO • SAN FRANCISCO SANTA BARBARA • SANTA CRUZ

JOHN C. HEMMINGER, DEAN
SCHOOL OF PHYSICAL SCIENCES
OFFICE OF THE DEAN

IRVINE, CALIFORNIA 92697-4675
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November 19, 2010

Professor Bruce C. Gates
Department of Chemical Engineering and Materials Sciences
University of California
3110 Bainer One Shields Avenue
Davis, CA 95616-5294

Dear Professor Gates:

The Basic Energy Sciences Advisory Committee (BESAC) has been charged by the Department of Energy Office of Science to assemble a Committee of Visitors (COV) to review the management processes for the Chemical Sciences, Geosciences, and Biosciences Division of the Basic Energy Sciences (BES) program. Thank you for agreeing to chair this BESAC COV panel. Under your leadership, the panel should provide an assessment of the processes used to solicit, review, recommend, and document proposal actions and monitor active projects and programs.

The panel should assess the operations of the Division's programs during the fiscal years 2008, 2009, and 2010. The panel may examine any files from this period for both DOE laboratory projects and university projects. The components of the Division that you are being asked to review are:

(1) Atomic, Molecular, and Optical Sciences
(2) Chemical Physics Research
(3) Catalysis Science
(4) Separations and Analyses
(5) Heavy Element Chemistry
(6) Geosciences Research
(7) Solar Photochemistry
(8) Photosynthetic Systems
(9) Physical Biosciences

You will be provided with background material on these program elements prior to the meeting. The COV is scheduled to take place on April 6-8, 2011 at the BES/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A presentation to BESAC is requested at its Summer 2011 meeting (as yet unscheduled). Following acceptance of the report

by the full BESAC committee, the COV report with findings and recommendations will be presented to the Director of the Office of Science.

I would like the panel to consider and provide evaluation of the following four major elements:

1. For both the DOE laboratory projects and the university projects, assess the efficacy and quality of the processes used to:
   (a) solicit, review, recommend, and document proposal actions and
   (b) monitor active projects and programs.
2. Within the boundaries defined by DOE missions and available funding, comment on how the award process has affected:
   (a) the breadth and depth of portfolio elements, and
   (b) the national and international standing of the portfolio elements.

In addition to the above elements, the panel is asked to provide input for the evaluation of Basic Energy Sciences progress toward the Government Performance and Results Act (GPRA) long-term goals (attached). Each of the components (or sub-components, if appropriate) of the Chemical Sciences, Geosciences, and Biosciences Division should be evaluated against each of the four GPRA long-term goals. If a particular long-term goal is not applicable to a specific program component, please indicate so in the evaluation. Note that the guidelines specify ratings of (1) excellent, (2) good, (3) fair, (4) poor or (5) not applicable. In addition to these ratings, comments on observed strengths or deficiencies in any component or sub-component of the Division's portfolio, and suggestions for improvement, would be very valuable.

If you have any questions regarding BESAC or its legalities, please contact Katie Perine, Office of Basic Energy Sciences at 301-903-6529 or by e-mail at katie.perine@science.doe.gov. Diane Marceau, the Program Analyst for the Chemical Sciences, Geosciences, and Biosciences Division, will provide logistical support for the COV meeting. She may be contacted by phone at 301-903-0235 or by e-mail at diane.marceau@science.doe.gov . For questions related to the Chemical Sciences, Geosciences, and Biosciences Division, please contact Eric Rohlfing, 301-903-8165, or by e-mail at eric.rohlfing@science.doe.gov . Also, if I can be of any help with the process, please feel free to contact me, 949-824-6020 or by email at jchemmin@uci.edu.

Sincerely,

John C. Hemminger, Chair
Basic Energy Sciences Advisory Committee

cc: H. Kung
E. Rohlfing
K. Perine
D. Marceau

Appendix B:

FY2011 Committee of Visitors Membership
Chemical Sciences, Geosciences, and Biosciences Division

Bruce Gates	COV Chair	University of California, Davis
AMO Sciences		
Tom Gallagher	Panel Lead	University of Virginia
Nora Berrah	Panelist	Western Michigan University
Nick Bigelow	Panelist	University of Rochester
Kate Kirby	Panelist	American Physical Society
Ron Phaneuf	Panelist	University of Nevada, Reno
Chemical Physics		
Veronica Vaida	Panel Lead	University of Colorado, Boulder
Michael Berman	Panelist	AFOSR
Ian Harrison	Panelist	University of Virginia
Anne McCoy	Panelist	Ohio State University
Hope Michelsen	Panelist	Sandia National Laboratory
Arthur Suits	Panelist	Wayne State University
Solar Photochemistry		
Jeanne Pemberton	Panel Lead	University of Arizona
Victor Batista	Panelist	Yale University
Dave Carlson	Panelist	BP Solar
Lin Chen	Panelist	ANL/Northwestern University
Matthew Platz	Panelist	NSF/Ohio State University
Biosciences		
Kay Simmons	Panel Lead	USDA
Carrie Harwood	Panelist	University of Washington
Julie Maupin-Furlow	Panelist	University of Florida
John Shanklin	Panelist	BNL
Cristina Ubach	Panelist	Monsanto
Catalysis Science		
Mark Barteau	Panel Lead	University of Delaware
Tom Baker	Panelist	University of Ottawa
Simon Bare	Panelist	UOP, LLC
Anne Chaka	Panelist	NIST
Nora Radu	Panelist	DuPont
Susannah Scott	Panelist	University of California, Santa Barbara
Heavy Element Chemistry/Separations and Analysis		
Rod Ewing	Panel Lead	University of Wisconsin
Laetitia Delmau	Panelist	ORNL
Laura Gagliardi	Panelist	University of Minnesota
Gordon Jarvinen	Panelist	LANL
Lloyd Smith	Panelist	University of Wisconsin
Geosciences		
John Valley	Panel Lead	University of Wisconsin
Patricia Maurice	Panelist	Notre Dame University
Katherine McCall	Panelist	University of Nevada, Reno
Kevin Rosso	Panelist	Pacific Northwest National Laboratory
Neil Sturchio	Panelist	University of Illinois, Chicago

Appendix C: **FINAL COV AGENDA**
Basic Energy Sciences Advisory Committee
Committee of Visitors for the
Chemical Sciences, Geosciences, and Biosciences Division
April 5-8, 2011

Tuesday, April 5, 2011				
Time	Activity	Committee Members	Division Staff	Location
6:30 PM	Informal Reception/Cash Bar	All	All	Bailey's
Wednesday, April 6, 2011				
Time	Activity	Committee Members	Division Staff	Location
7:30 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
8:30 AM	Welcome and Charge to the Committee	All	John Hemminger, Chair Basic Energy Sciences Advisory Committee	A-410
8:40 AM	Overview of Basic Energy Sciences	All	Harriet Kung, Director, Office of Basic Energy Sciences	A-410
9:00 AM	Overview of the Chemical Sciences, Geosciences, and Biosciences Division	All	Eric Rohlfing, Director, Chemical Sciences, Geosciences, and Biosciences Division	A-410
9:30 AM	Update on the SC Portfolio Analysis and Management System (PAMS)	All	Linda Blevins, Office of Science	A-410
9:50 AM	Review procedures	All	Rich Greene, Team Lead, Photo- and Biochemistry	A-410
10:15 AM	Instructions and Schedule	All	Bruce Gates, Chair, Committee of Visitors	A-410
10:30 AM	Break and disperse to panel rooms			
10:45 AM	**First Read Panel 1** Atomic, Molecular, and Optical Sciences	**Gallagher** Berrah, Bigelow Kirby, Phaneuf	Jeff Krause	A-410
10:45AM	**First Read Panel 2** Chemical Physics	**Vaida,** Berman Harrison, McCoy Michelson, Suits	Wade Sisk Greg Fiechtner Mark Pederson	E-401
10:45AM	**First Read Panel 3** Solar Photochemistry	**Pemberton,** Batista Carlson, Chen, Platz	Mark Spitler Amy Ryan (detailee)	F-441

10:45AM	**First Read Panel 4** Biosciences	**Simmons,** Harwood Maupin-Furlow, Shanklin, Ubach	Gail McLean Bob Stack	G-426
10:45 M	**First Read Panel 5** Catalysis Science	**Barteau,** Baker Bare,Chaka Radu, Scott	Raul Miranda Paul Maupin Jan Hrbek (detailee)	E-301
10:45AM	**First Read Panel 6** Heavy Element Chemistry Separations and Analysis	**Ewing,** Delmau Gagliardi, Jarvinen Smith	Larry Rahn	E-114
10:45AM	**First Read Panel 7** Geosciences	**Valley,** Maurice McCall, Rosso Sturchio	Nick Woodward	G-207
12:30PM	Working Lunch	All	All	A-410
1:30 PM	**Resume First Read Panels**	Panels		Panel Rooms
4:00 PM	**Preliminary Report Drafting—Key Elements and Gaps**	Panels		Panel Rooms
5:00 PM	Meeting between Panel Leads and Chair	Panel Leads and Chair		A-410
5:30 PM	Meeting with Chair and BES Senior Management	Chair	Harriet Kung, Eric Rohlfing	A-410
5:45 PM	Return to Hotel	All	Drivers with Cars or walk	A-410
6:30 PM	Pickup at Hotel for Transport to Dinner	All	Drivers with Cars	
7:00 PM	Dinner for COV and BES Staff	All	All	That's Amore

Thursday, April 7, 2011				
Time	**Activity**	**Committee Members**	**Division Staff**	**Location**
7:30 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with Cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
8:30 AM	Fundamental Interactions Team Session	Panels 1 and 2	Michael Casassa Wade Sisk Greg Fiechtner Mark Pederson	E-401

8:30 AM	Fundamental Interactions Team Session	Panels 3 and 4	Rich Greene Mark Spitler Carol Bessel Gail McLean Bob Stack Amy Ryan (detailee)	G-426
8:30 AM	Fundamental Interactions Team Session	Panels 5, 6, and 7	John Miller Raul Miranda Paul Maupin Jan Hrbek (detailee) Larry Rahn Nick Woodward	E-301
9:15 AM	Complete First-Read Panel Reports	Panels		panel rooms
11:15AM	COV Executive Session Panel Lead Reports	All		A-410
12:30 AM	**Lunch**	**All**		A-410
12:30 PM	**Working Lunch**	**Chair and Panel Leads**		Chair Headquarters
1:30 PM	**Second Read Panel 1** Atomic, Molecular, and Optical Sciences	**Gallagher,** Baker Berman, Chen Rosso	Jeff Krause	A-410
1:30 PM	**Second Read Panel 2** Chemical Physics	**Vaida,** Berrah Carlson, Chaka McCall, Sturchio	Wade Sisk Greg Fiechtner Mark Pederson	E-401
1:30 PM	**Second Read Panel 3** Solar Photochemistry	**Pemberton,** Gagliardi Harwood, Kirby Suits	Mark Spitler Amy Ryan (detailee)	F-441
1:30 PM	**Second Read Panel 4** Biosciences	**Simmons,** Maurice McCoy, Smith	Gail McLean Bob Stack	G-426
1:30 PM	**Second Read Panel 5** Catalysis Science	**Barteau,** Batista Delmau, Harrison Maupin-Furlow, Phaneuf	Raul Miranda Paul Maupin Jan Hrbek (detailee)	E-301
1:30 PM	**Second Read Panel 6** Heavy Element Chemistry Separations and Analysis	**Ewing,** Bigelow Scott, Ubach	Larry Rahn	E-114

1:30 PM	**Second Read Panel 7 Geosciences**	**Valley,** Jarvinen Michelsen, Radu Shanklin	Nick Woodward	G-207
4:00 PM	Merge First and Second Read Input Finalize Draft Panel Reports/ Formulate points for report	First Read Panels		Panel Rooms
5:30 PM	Return to hotel	All	Drivers with Cars or Walk	A-410
	Dinner on your own	All	None	
Friday, April 8, 2011				
Time	**Activity**	**Committee Members**	**Division Staff**	**Location**
7:30 AM	Travel from Fairfield Inn to DOE Germantown	All	Drivers with Cars	Fairfield Inn Lobby
8:00 AM	Continental Breakfast Available	All		A-410
8:20 AM	COV Executive Session	All		A-410
9:15 AM	Closeout Session with COV and BES Staff	All	All	A-410
10:00 AM	COV Chair meets with BES Senior Management	COV Chair	Harriet Kung Eric Rohlfing	A-410

Appendix D: **FIRST-READ/SECOND-READ/MERGE REPORT TEMPLATE (Illustrated for Panel 1)**

Panel 1: Atomic, Molecular, and Optical Science

BES COMMITTEE OF VISITORS (COV)
Reviewing the Chemical Sciences, Geosciences, and Biosciences Division
Fiscal Years 2008, 2009, and 2010

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 program'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
- effective interactions between program managers and PIs

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 and BES
- the relevance of the portfolio with respect to the missions of the program, division, BES, and DOE
- 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). For each goal, adjectival ratings are defined and a template for rating each goal is provided.

1. 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.

> **Excellent** – BES-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.
> **Good** – BES-supported research leads to a steady stream of outputs of high quality.
> **Fair** – BES-supported research leads to modest outputs of good quality.
> **Poor** – BES-supported research leads to limited outputs.
> **Not Applicable** – the goal is not applicable to the program(s) under review.

Progress rating for the program under review (select one):

> __ Excellent
> __ Good
> __ Fair
> __ Poor

Comments:

2. 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.

> **Excellent** – BES-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.
> **Good** – BES-supported research leads to a steady stream of outputs of high quality.
> **Fair** – BES-supported research leads to modest outputs of good quality.
> **Poor** – BES-supported research leads to limited outputs.
> **Not Applicable** – the goal is not applicable to the program(s) under review.

Progress rating for the program under review (select one):

__ Excellent
__ Good
__ Fair
__ Poor

Comments:

3. Develop new concepts and improve existing methods for major energy research needs identified in the 2003 Basic Energy Sciences Advisory Committee workshop report, Basic Research Needs to Assure a Secure Energy Future.

Excellent – BES-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.
Good – BES-supported research leads to a steady stream of outputs of high quality.
Fair – BES-supported research leads to modest outputs of good quality.
Poor – BES-supported research leads to limited outputs.
Not Applicable – the goal is not applicable to the program(s) under review.

Progress rating for the program under review (select one):

__ Excellent
__ Good
__ Fair
__ Poor

Comments:

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Excellent – BES-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.
Good – BES-supported research leads to a steady stream of outputs of high quality.
Fair – BES-supported research leads to modest outputs of good quality.
Poor – BES-supported research leads to limited outputs.
Not Applicable – the goal is not applicable to the program(s) under review.

Progress rating for the program under review (select one):

__ Excellent
__ Good
__ Fair
__ Poor

Comments:

Appendix E: FINDINGS, COMMENTS, AND RECOMMENDATIONS OF INDIVIDUAL PANELS INCLUDING PANEL RATINGS OF PROGRESS TOWARD LONG-TERM BES GOALS

The detailed findings, comments, and recommendations of each panel presented below were not discussed fully by the COV as a whole, although all COV members had the opportunity to comment on all of the summaries of the panels' findings and recommendations in their discussion of the emerging draft COV report. Many of the findings and recommendations common to more than one panel were discussed in the COV meeting on Thursday and \ Friday and with CSGB Division Management and Staff on Friday.

Panel 1: Atomic, Molecular, and Optical Sciences

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

The panel judges that the review process is thorough and professionally executed by the Program Manager. Funding decisions are well substantiated on the basis of reviews, programmatic considerations, and the maintenance of balance in the overall program portfolio. Files containing all the relevant communications and documents are well maintained. The contents of these files demonstrate commendable levels of communication between principal investigators and the Program Manager, with good feedback to principal investigators.

An extensive international pool of highly qualified reviewers is employed to assess proposals. A thorough peer-review process is followed (with typically 5-6 reviews per proposal). Proposals from the National Laboratories are definitely becoming more forward looking, consistent with the recommendation of the COV that met three years ago. The average interval between proposal submission and funding is 6 ± 3 months for a sample of 11 proposals. This interval is commendable given the number of reviews and budget uncertainties.

Comments and Recommendations:

The panel suggests requiring white papers for potential new proposals and keeping track of them. This procedure will have several benefits, including more meaningful statistics regarding proposal pressure and success rates and reduction of the number of proposals that are "dead-on-arrival" for programmatic reasons (such proposals waste substantial Program Manager and reviewer time). The panel suggests sending several related proposals to the same reviewer at one time to obtain a relative ranking and ensuring that each proposal be reviewed by at least one nonspecialist to provide a more general review. Proposals from the National Laboratories should be more uniformly prospective than they typically are, and should provide more details of the proposed work than they typically do.

(b) Monitor active project and programs

Findings:

The regularity and rigor of the periodic review process (specifically, the principal investigator meeting and the abstracts submitted for it) provide valuable portfolio assessment tools for the Program Managers and feedback to principal investigators about their roles in the program.

Comments and Recommendations:

The panel recommends more site visits to individual principal investigators by the Program Managers and more travel by the Program Managers to important national and international conferences.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

The program is aligned with recognized frontiers in atomic, molecular, and optical science that are consistent with the overall DOE mission (including ultra-fast and correlated processes and quantum control of atoms and molecules). The program shows a commitment to support research conducted at DOE National Facilities (primarily light sources). Interdisciplinary research is conducted both in projects carried out by individual principal investigators and National Laboratory programs. The continuing shift of the BES Atomic, Molecular, and Optical Sciences portfolio represents a significant degree of innovation with a moderate and appropriate level of risk. A predominant theme of the program is creating, controlling, and analyzing matter at the atomic and molecular level, and research on this theme underpins and enables research in other disciplines and energy-related applications. The program is characterized by an appropriate mix of experiment, theory, and modeling.

New programs comprise 16% of AMOS portfolio during the review period.

The funding provided for single investigator grants is marginal for most of the BES Atomic, Molecular, and Optical Science program.

Recommendations:

Remaining impediments, if any, to the funding of related research programs by multiple agencies should be reduced.

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

Findings:

The significance and broad impact of the Atomic, Molecular, and Optical Sciences research program are evidenced by impressive numbers of publications in high-profile journals such as *Science*, *Nature*, and *Physical Review Letters*. Among the principal investigators in the program are: National Academy of Sciences members; 60 American Physical Society fellows; and winners of the McArthur, Rabi, Wood, Schawlow, Zewail, Davisson-Germer, Langmuir, Plyler, Ives, and Alexander von Humboldt Foundation prizes and awards.

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

1. 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:

Excellent

Comments:

The Atomic, Molecular, and Optical Sciences program develops fundamental understanding upon which new technologies for energy conversion can be developed.

2. 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:

Excellent

Comments:

The program addresses control at the molecular level involving all phases of matter.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

The research in the program is exploring new techniques to understand and control all phases of matter at the quantum level. This work contributes an atomistic approach to understanding of reaction pathways and the foundations of energy transfer, conversion, and storage.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:
Excellent

Comments:

The program continues to develop novel sources of photons, ions, and electrons to probe and control matter, providing enhanced fundamental understanding of chemical reactions.

Panel 2: Chemical Physics

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

The panel concludes that the Program Managers do an excellent job of distilling reviews and summarizing the thought process for their decisions summarized in the selection memos. Typically, each submission is read by 5-6 reviewers. These reviewers cover an appropriate range of expertise, nationalities, and backgrounds. The overall quality of the reviews is very high. The program officers are commended for finding groups of individuals who provide detailed, nuanced reviews.

Comments:

The diversity of the reviewers in terms of expertise and nationality is applauded. The panel noted that whereas reviews of proposals from universities were provided in a timely manner, it took longer for replies following visits to reach the national laboratories.

The panel looks forward with enthusiasm to the full implementation of the new database system (PAMS).

Recommendations:

The panel encourages even more inclusion of un-funded and young potential new investigators at the principal investigator meetings. Conversations between funded investigators and Program Managers need to take place, especially with respect to research directions and changes in program missions. The Program Managers are encouraged to ensure that appropriate guidance is given to a principal investigator if his/her funding is in danger, especially when the work is of high scientific quality.

Explicit solicitations would be useful in making the pre-proposal process more transparent. The panel suggests explicit solicitations of research proposals with a more formalized structure of handling the initial inquiries. The SISGR model provides an excellent model—are there possibilities for expanding this procedure to other announcements?

The panel looks forward to the time when Program Managers will be able to take advantage of the new database system (PAMS) to keep track of initial contacts with potential principal investigators as well as the recommendations and outcomes of white papers.

(b) Monitor active project and programs

Findings:

The panel finds that monitoring of the progress of projects is well documented. The Program Managers have found mechanisms to increase participation of un-funded investigators at the principal investigators' meetings.

Site visits to laboratories are valuable; the formal feedback from laboratory site visits can take more than a year.

Recommendations:

The panel recommends more frequent feedback and advice from the Program Managers to the principal investigators, particularly those at National Laboratories, regarding mid-course corrections in research.

We recommend shorter turn-around times for reviews of the Laboratories from the Program Managers.

Site visits to National Laboratories are valuable and could be extended to include universities, especially for multi-PI proposals or when there are multiple PIs at a single institution. It is also recommended that the Program Managers attend more scientific meetings to obtain a broader view of the current issues and interact with scientists outside of the program.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

The overall quality of the science is exceptional. The appropriateness of the scope and funding level is limited by resources. The SISGR, Midscale Instrument, and Chemical Imaging Programs provide valuable flexibility to fund new innovative and high-risk proposals

BES is making advances in cooperative planning with other parts of DOE (e.g., EERE), and CTC has been collaborating with ASCR.

Comments:

There is a challenge with respect to finding the "balance of projects with respect to innovation, risk, and interdisciplinary research" and educating the reviewers on this aspect of the mission.

SISGR provides an innovative model for expanding the group of PIs by using a solicitation scheme arising from the 2003 COV Report.

Recommendations:

Revise instructions to reviewers to encourage them to consider the balance of the project with respect to innovation, risk, and interdisciplinary research.

Program Managers should consider extending the award duration of highly rated proposals to reduce administrative burden.

More calls for proposals for midscale instrumentation are encouraged, and barriers for collaboration between the fundamental and the applied programs in DOE should be lowered.

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

Findings:

The stature of the principal investigators supported by BES (and the reviewers) is very high, as indicated by their international standing.

The program is unique, particularly with respect to (1) program focus and (2) capabilities and user facilities.

Comments:

The National Laboratories are an extremely valuable component of the BES research programs, unique in the world.

Recommendations:

Maintain the state-of-the-art National Laboratory facilities and support researchers who use them.

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

1. 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:

Excellent

Comments:

Some outstanding examples supporting the rating include the following: (a) Determination of design principles for optimizing (via quantum mechanics) new materials for efficient and inexpensive photovoltaic devices, (b) characterization of O_2 adsorption on single-component and alloy metal nanoparticles for catalysis, (c) new theoretical and computational methods used to develop materials for carbon capture, and (d) exquisite characterization and analysis of bio-macromolecules resolving effects of chemical fluctuations and chemical environments.

2. 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:

Excellent

Comments:

The programs are active and evolving, with important topics in active areas including high-pressure combustion; isomer-specific reactivity and dynamics; soot formation and growth; novel free radical detection; and predictive modeling of internal combustion engines.

Studies in these programs generate unique, high-impact results. Principal investigators develop sophisticated methods spanning the range from quantum calculations of individual reaction rates to large kinetics models. Many BES principal investigators make use of DOE user facilities to produce surprising, high-impact interdisciplinary results. Principal investigators create highly accurate, state-of-the-art potential energy surfaces for polyatomic systems that have yielded fundamental new insights into chemical reactivity.

Specific examples include the following:

- Isomerization dynamics from a variety of experimental perspectives.
- Characterization of new mechanisms of chemical reactions.
- Development in CCSD(T) methodologies and their applications to combustion processes.
- Experiment/theory collaborations in investigations of mechanisms of electronic excitations at surfaces.

The program funds a broad range of leading scientists who are exploring processes at surfaces by using a variety of experimental and theoretical approaches, including quantum/classical dynamics; examining carbon capture at interfaces; and single-molecule spectroscopy to probe electron transfer processes. Examples of projects in surface processes include the following:

- Theoretical studies of clusters and nano-particles for energy conversion.
- Investigation of the structure/function relationships in catalysis by nano-sized structures.
- Modeling of electron transport in energy conversion schemes.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

Of the 10 general research directions suggested in the 2003 report "Basic Research Needs to Assure a Secure Energy Future," the Chemical Physics Division is providing important molecular-level understanding of fundamental processes relevant to at least six of these 10 research directions/needs, that is, materials science to transcend energy barriers, basic research towards a hydrogen economy, innovative energy storage, heterogeneous catalysis, fundamental approaches to energy conversion, and basic research for energy utilization efficiency.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

The program has demonstrated progress in developing unique instrumentation for many novel applications, including the following:

- Probing electronic and molecular structures with high spatial or temporal resolution at surfaces (e.g., STM, transient absorption spectroscopy) and in the gas phase (e.g., Rydberg fingerprinting).
- Imaging vibronic states with sub-nanometer resolution.
- Single-molecule spectroscopies.
- Use of the ALS for probing microscopic details of mechanisms and dynamics, new high-resolution spectroscopic tools, and chemical imaging.

- Ultrafast X-ray spectroscopies.

Decisions by Program Managers are thoughtful and well informed.

Panel 3: Solar Photochemistry

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

The focus of this program and the specific mission are sometimes not transparent enough, especially for new investigators (and also for current principal investigators when there are changes in the scope and/or mission of the program). Information on the website is generally very good, but it does not emphasize the fundamental research focus of the program, as opposed to device-oriented developmental work. This is the only program with "solar" in its name, and so this distinction is critical for the program to generate the proposals it seeks and to minimize proposals that should be directed to other parts of DOE.

The use of the informal white paper route is very effective in terms of minimizing proposal pressure and reviewer workload. The panel was somewhat concerned about whether this filter of a single individual may eliminate some worthy high-risk, high-impact ideas.

The timing of proposal review and award decisions was considered to be excellent.

For the most part, the reviewers chosen for proposals were excellent and had the appropriate expertise to provide informed, well-reasoned, in-depth reviews.

A few questions arose about why some proposals were not funded for programmatic reasons; the reasons did not seem to be clearly documented in all cases.

The use of the checklists on the fronts of folders seems somewhat uneven in that not all the steps included on the checklist were used and dated. One or two folders seemed incomplete. In one instance, for example, the selection memo states that five reviewers were used, but only three reviews were included in the folder.

The National Laboratory site visits appear to be very effective; the corresponding reviews were thorough and thoughtful. The panel judged that good decisions are being made regarding National Laboratory FWP proposals. The panel clearly sees a positive response to the recommendation by the 2008 COV to take more account of the plans for research and not just a review of accomplishments. This emphasis on prospective reviews was clearly noted in the recent reviews.

The panel considered several cases of funded proposals receiving a single negative review with otherwise favorable reviews; the panel questioned whether additional reviews from individuals with expertise similar to that of the person providing the negative review were solicited prior to a decision.

Comments:

The panel questioned the use of different rating scales for different solicitations and the absence of a requested rating scale for proposals for continuing research; would it be useful for a single rating scale to be used for all proposals? Is there a reason why different rating scales (or none) are used inconsistently?

The panel questioned the balance between reviewers from those already funded by the program and those not funded by the program. In a sense, those already funded by the program could be perceived as potentially being in conflict, because they are competing for the same resources, although admittedly they have excellent, relevant expertise. The panel wondered whether enough "at arms' length" reviewers were sought.

Recommendations:

The program is encouraged to provide more program-specific guidance to proposers regarding the nature of the scientific activities funded; the structures desired for various submissions (including white papers and proposals); the specific sections to be included in white papers and proposals; and the specific types of scientific activities for which funding might be provided. Greater clarity in this regard might make the process more transparent to proposers, especially those new to the program.

New applicants should be strongly encouraged to attend the annual principal investigators meeting, or initiate collaborations with current members of the program, to learn about the problems, questions, scope, and collaborative structure of existing research projects and thereby have the opportunity to be more successful.

(b) Monitor active project and programs

Findings:

It is clear that the program is actively managed in an effective way. The expertise of the Program Manager in the scientific areas that are the focus of this program is excellent and contributes substantially to the success of this program.

The role and use of written annual reports in portfolio decision-making is not clear. These reports take on quite different forms and are of various depths and scope. It may be useful to provide more structured guidelines for preparation of these reports. No comments evaluating annual reports are included in the folders. It is not clear to the panel how these are used other than as a step in the release of the next year's funding.

Comments:

The continuity of the Program Managers in the Solar Photochemistry program has been good and is important to the long-term success of the program. The panel expresses the hope that the current Program Manager will be in place as long as the preceding Program Manager.

The panel commends the Program Manager's excellent efforts (and those of his predecessor) in maintaining statistics about this program; this data collection is above and beyond expectations in the absence of a regular data management system within BES.

This program has a significant component of work accomplished by small groups of faculty. The need for and use of instrumentation by these small groups is very high. A sustainable mechanism for funding this needed instrumentation that does not negatively impact the ability of this program to support continuing expenses associated with the work of these groups needs to be found.

Recommendations:

As part of the COV evaluation of program impact, it might be useful to broaden the opportunity for community input regarding program impact through creation of a website for soliciting anonymous feedback. This feedback could then be used as part of the information stream provided to the COV for their analysis.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

The panel was favorably impressed with information provided that indicated the regular inclusion of new investigators, keeping the program vibrant and progressive.

The portfolio is mission-focused, but for some of the basic research activities, the connection between the work and the mission is not always clearly articulated.

The balance between maintaining expertise and bringing in new investigators seems to be good, although the high-risk aspects of the program's efforts do not clearly stand out.

The panel notes that the Solar Photochemistry program deserves recognition for the success of many of the solar-based Energy Frontier Research Centers (which are outside the scope of this review); many of the investigators in these centers have been previously funded by the Solar Photochemistry program, and it is the growth and maintenance of the expertise supported by this program over many years that led in a significant way to the evolution of these Centers based on this fundamental science.

The panel was favorably impressed by the strong synergy in the Solar Photochemistry program that has arisen as a result of the reorganization of this program into the Photo- and Bio-chemistry Team.

The Program Manager has successfully managed the transfer of some funded activities to more appropriate programs. The Program Manager is encouraged to continue to actively manage such programs that evolve to be at the interface with other programs (e.g., Catalysis, CPIMS).

Comments:

It could be possible that some would perceive a tension between the fundamental research in the solar and photochemistry program and the device development supported by other parts of DOE (e.g., EERE and the Energy Frontier Research Centers). Such perceptions must be carefully managed; it is important to convey the synergy between these programs rather than any potential competition or any perception of redundancy. The interface and formal communication between the basic science and applied programs must be managed and facilitated, with an effort to demonstrate how the fundamental science is distinct from applied work and complementary to it.

Recommendations:

The panel wonders whether there might be a positive role for some independent group as a coordinating body for developments in solar-based energy technologies nationwide, including those funded by various segments of DOE. The function of this group would be to maintain a big-picture view of the nation's progress in these technologies in comparison with competitive international efforts, to monitor potential synergies and unnecessary redundancies between U.S. programs, and to promote communication between various groups who are stakeholders in solar-based energy technologies.

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

Findings:

The principal investigators funded in the program are scientists of high stature or are newly emerging stars. This program supports a well-established community whose members continue to make significant contributions to the evolution of this science.

Comments:

It is not clear how U.S. efforts in solar photochemistry are benchmarked in terms of progress on an international scale. There is no clear design of an international component of the efforts of this program, nor is it clear how the Program Manager can stay fully abreast of international developments in the field, especially those occurring in countries that are emerging as major players in the area such as China.

Recommendations:

Funding for Program Managers to participate in national and international meetings is essential.

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

GENERAL COMMENT:

The panel wonders, in an era of budgets based on continuing resolutions, how meaningful it may be to assess progress by GPRA metrics when the means to achieve the goals are not provided.

1. 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:

Excellent

Comments:

This program's efforts are clearly (and appropriately) focused on the molecular scale more than the nanoscale, although many funded efforts are clearly related to the use of nanoscale materials. Use of biomaterials is also evident in this program.

2. 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:

Excellent

Comments:

This aspect of energy research is strongly embedded in this program's mission.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

These aspects of the mission are clearly embedded in this program's activities.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

Advances in instrumentation and instrumentation use are apparent in the program's portfolio, although it is more difficult to ascertain the level of use of large instrumentation by academic scientists than by National Laboratory scientists.

PANEL 4: Biosciences

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

Timely solicitation of proposals from the science community has been effectively continued and has resulted in applications both from scientists new to the program and from those with continuing projects. The two-part review process (involving pre-proposals followed, upon encouragement, by full proposals) has entailed extensive internal screening, yielding well-developed full investigator proposals in areas appropriate to the mission of the program. Examination of the jackets of proposals that were funded or declined shows outstanding compliance to the process. Decisions are well justified, demonstrating the enormous diligence of the Program Managers regarding documentation for both approved and declined proposals.

Comments:

Excellent leadership at BES ensures that principal investigators are empowered to effectively steward their programs. The panel included an excellent representation of experts funded by the program and experts not funded by the program. The COV panel wonders whether a short-term solution could be developed to ensure timely extractions of proposals from grants.gov.

Recommendations:

The panel strongly endorses the present process involving pre-applications and full proposal reviews as well as the single annual deadline for full proposal submission and face-to-face panel meetings for the review process.

It is recommended that Program Managers should consider expanded use of four-year grants.

Ample resources should be provided for Program Managers to travel to meetings, conferences, and workshops.

The panel encourages Program Managers to ensure that their websites are easily accessible and that the vision and programmatic goals are clearly articulated.

(b) monitor active project and programs

Findings:

Principal investigator meetings have been established and are highly successful with respect to interactions between principal investigators and as a forum for Managers to convey programmatic themes.

Program Managers do an effective job of monitoring progress through progress reports, principal investigator meetings, direct contacts with principal investigators by telephone, and attendance at scientific meetings.

A strong and successful effort has been made to more fully integrate the program with other programs in BES, especially the physical and chemical sciences, with a positive trajectory in this direction.

Site visits are an effective and important mechanism for monitoring the progress of multi-investigator programs.

Comments and Recommendations:

The panel looks forward with enthusiasm to the rapid implementation of the data management system (PAMS) and suggests development of an interim method to transfer proposals from grants.gov to a compiled form that is useful for Program Managers.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

Program Managers have formulated a clear vision of the direction of the program. This program has had great success in funding fundamental research that has evolved into central themes in plant and microbial biology.

The program has evolved over the past three years to become more closely aligned to the DOE mission. The Photosynthetic Systems program is the thriving nexus for natural photosynthesis research.

Science funded by previous Biosciences awards has been leveraged to establish more applied, high-impact initiatives such as the DOE Energy Frontier Research Centers, the DOE Bioenergy Centers, and private-sector initiatives.

Recommendations:

None

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

Findings:

The quality of publications emerging from research supported in the program has been exceptional during this transition to an increased focus on energy. The principal investigators are publishing in top-tier, high-impact research journals; this group includes 18 members of the National Academy of Sciences, 47 fellows of AAAS, and a number of winners of prestigious awards.

Recommendations:

None

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

1. 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:

Excellent
Comments:

Examples of progress in interfacing living and non-living systems at the nanoscale include attachment of living cells to devices for biohydrogen production and microbial fuel cells. Scientists at the Center for Plant and Microbial Complex Carbohydrates have made substantial

progress in characterizing cell wall synthesis and assembly which serves as the basis for understanding complex plant materials with potential use in bioenergy production. Recent work was carried out to understand structure-function relationships in natural photosynthetic systems for the design and optimization of novel biohybrid systems.

Recommendations:

See composite recommendations at end of this section.

2. 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:

Excellent

Comments:

Research led to redesigned enzyme activities and successful application to metabolically engineered plants to accumulate industrially relevant yields of tailored biomaterials such as omega 3-fatty acids for renewable industrial applications.

New approaches in X-ray spectroscopy were developed for understanding of mechanisms of water oxidation and oxygen evolution catalyzed by PSII in its natural orientation within membrane samples.

Recommendations:

See composite recommendations at end of this section.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

Super-resolution characterization of natural photosynthesis led to understanding of how green plants and algae regulate the efficiency of light harvesting in PSII. This knowledge could lead to strategies for improving photosynthetic efficiency.

Evidence was presented for a novel form of energy conservation that leads to CO_2 conversion into methane. This mechanism (called electron bifurcation) is likely widely used in biology.

Recommendations:

See composite recommendations at end of this section.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

A new method (termed fluctuation solution X-ray diffraction) was developed for *in-situ* study of membrane proteins in solution without crystallization.
Cutting-edge solid-state NMR spectroscopy was applied to investigate structure and dynamics of light harvesting complex 1 of *R. sphaeroides*. The techniques are particularly well suited to investigation of dynamic disordered protein complexes.

Recommendations (for III. 1-4):

The panel endorses these types of interdisciplinary research; continued leveraging of and cross fertilization between Energy Biosciences and other BES programs and federal agencies; and continued investment in high-risk, high-reward projects, for example, to elucidate protein dynamics and the structure of membrane proteins.

Panel 5: Catalysis Science

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

Catalysis plays a role that is central to DOE's mission. The report "Basic Research Needs: Catalysis for Energy" provides a valuable roadmap for the field, and the National Academy of Sciences Report "Catalysis for Energy: Fundamental Science and Long-Term Impacts of the U.S. Department of Energy Basic Energy Sciences Catalysis Science Program" demonstrates the excellent quality of the program and impressive growth in funding of new principal investigators during the review period. The assessment for the current period is well aligned with the conclusions of the more detailed National Academy of Sciences report.

The Program Managers used good decision making processes; reviews were thorough and well summarized in the funding recommendations. There has been good use of mail-in reviews to supplement on-site reviews for the National Laboratories. The time to return decisions on proposals was in the range of 3–11 months, considered by this panel to be appropriate.

The BES staff is highly competent, and the new PAMS system will make them even more effective.

The white paper process with its rapid turn-around works very well in the Catalysis program. The risk is that good new ideas may be discouraged by a too-narrow perspective of a sole Program Manager (or a new Detailee), as the success depends on the perspective and experience of the Program Manager. The Catalysis program has an advantage over others in BES, as it has two permanent Program Managers and one Detailee, who work very well together. Continuing success and sustainability in the program is critically dependent on having Program Managers with a broad and forward-looking perspective that is not too narrow to encourage an influx of new ideas and new principal investigators.

Comments:

For University Awards

The funded proposals had generally very strong reviews, and the funding decisions were well justified. Decline of proposals was also generally well justified. The number of reviews was always three or more. Some multidisciplinary proposals were skewed toward other fields, but were funded or split-funded by the Catalysis Science Program, showing the broad view of Program Managers. Large multi-investigator proposals did (appropriately) get more reviews. The length and thoroughness of reviews varied significantly, and it appears the Program Managers weighted them appropriately. The panel commends the involvement of non-U.S. reviewers.

The panel is concerned about the relatively low termination rate.

For National Laboratory Awards

The panel sees evidence of the intent of laboratory management to take appropriate action based on reviews in almost all cases. There was, however, one example of a renewal proposal that received poor reviews and was funded.

The panel judges that there is a benefit to having the site visitors receive some of the mail review input in some fashion. The current practice of the Program Manager conveying the information to the on-site panel is effective.

Recommendations:

The panel judges the white-paper process to be invaluable for identifying new ideas and principal investigators, and judges that it should be institutionalized in some manner (it does not need to be formal).

The panel encourages the involvement of more industrial reviewers.

Recognizing the progress being made with PAMS, the panel looks forward to its implementation and recommends that BES consider using PAMS to better track trajectories from contact to white paper to initial proposal and beyond.

With the trend toward large multi-principal investigator grants, site visits should increasingly be part of the program evaluation.

Participation of Program Managers in a wide range of scientific meetings is critical to maintaining and enhancing broad and forward-looking perspective at BES.

The panel recommends that instructions for informal pre-proposal contacts be prominent on the BES website.

The panel recommends that BES consider transitioning to four-year awards for renewals to reduce administrative overhead.

The PAMS system should be designed for responsiveness to federal-wide efforts to build an information base suitable for tracking the impact of program support (e.g., STAR METRICS).

(b) Monitor active project and programs

Findings:

The staff uses opportunities for principal investigator meetings and international conferences well, but needs to attend more of them. The staff makes use of a broad range of formal and informal interactions with principal investigators. Site visits produce important perspectives on leadership and synergy of laboratory/large programs that could not be obtained via mail reviews.

Recommendations:

Scientific conferences should be used to identify a broader base of reviewers, particularly those from industry.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

There is evidence of clear and strong communication between the Program Managers at BES and their counterparts at other agencies, particularly NSF, and the panel commends these interactions.

The National Academy of Sciences report was useful to the panel for the international context it provides and for its assessment of the impact of BES-supported research. However, there is concern that DOE's support for catalysis, although generous, is not keeping pace with international investment in the field.

The portfolio quality that the panel examined is excellent, and the program supports work important to the advancement of the field. Superb new investigators were added to the program. The program has an appropriate emphasis on tool development.

Comments:

There is a strong potential for synergy between the Catalysis program and selected EFRC programs.

The panel found that the chemical transformations panel session (combining Panels 5, 6, and 7) was helpful, providing useful information about how the funding balance is decided, the relationship between new funding and new principal investigators, and networking with Program Manager counterparts in other agencies.

Recommendations:

The panel recommends that synergy be promoted between the Catalysis program and related EFRCs. For example, in the future the EFRC COV might be timed to coincide with and/or have common members with the COV evaluating the Catalysis program, perhaps at the first opportunity (but the panel recognizes that scheduling constraints and legal requirements for the COV activities may make it difficult to implement this recommendation).
If the funding period for renewals is not extended to four years, then timely merit-based extensions should be considered.

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

Findings:

As demonstrated in the National Academy of Sciences report and confirmed by the panel's review, the program funds visible, high-impact researchers who are recognized leaders in their fields. Continuity of funding has been an important contributor to program impact.

About 50% of the program's budget increase since 2001 has supported new investigators; this trend is highly commendable.

Recommendations:

It is important to continue to welcome and solicit ideas for high-risk research to maintain leadership in the field.

The Catalysis program is a model of working at the interface between disciplines and should be considered a model for other BES programs.

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

1. 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:

Excellent

Comments:

The panel judges that the rating for progress is excellent. The progress in synthesizing and characterizing static structures is well advanced; the panel is encouraged to see that the future emphasis is on dynamic structures of catalysts under working conditions.

2. 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:

Excellent

Comments:

Progress is excellent, particularly with theory being well integrated into many projects. The Catalysis program has been a leader in integrating theory and experiment. Continuing efforts need to facilitate greater crosscutting interactions between disciplines, such as more interdisciplinary principal investigator meetings.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

The 2008 Basic Research Needs report Catalysis for Energy provides concrete methods to accomplish this goal. The program is doing an excellent job of following this roadmap within a broader portfolio of activities needed to advance the field within budget constraints.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

This commitment is primarily expressed through the large National Laboratory facilities such as LCLS, SNS, TEAM, SSRL, APS, and the NSLS-II project. These are all world-leading facilities. The call for instrumentation proposals from universities is a good start for supporting new instrumentation, and the panel encourages continuation of the opportunity.

The Synchrotron Catalysis Consortium at NSLS is a good example of how BES increases the impact and accessibility of a large user facility to advance catalysis research. Representatives from such user facilities should be encouraged to present the capabilities at principal investigator meetings.

Panel 6: Heavy Element Chemistry/Separations & Analysis

I. EFFICACY AND QUALITY OF THE PROGRAM'S PROCESSES

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

Findings:

In the judgment of the panel, the review process works very well, resulting in a substantive and distinguished portfolio of excellent science. Reviews are conducted carefully by highly qualified reviewers, including some excellent reviewers from abroad. A greater effort might be made to draw on reviewers outside of the community of researchers, particularly in the Heavy Element Chemistry part of the program.

The evaluation process and the basis for the funding decisions are generally very well documented. In some cases, particularly for the National Laboratories, programmatic or institutional considerations have an impact on the final decision.

The process works well because of the attention and efforts of the Program Managers. Because of the importance of their judgment, they are critical to the success of the process.

It is imperative that the Program Managers remain in close contact with the scientific community they serve.

The data management system that is being implemented by the Office of Science (PAMS) will be an important tool for the staff in managing the entire review and funding process and will support their monitoring of program progress and the identification of programmatic needs; it is enthusiastically welcomed.

Comments and recommendations:

The process of using white papers as an initial screening tool is much welcomed. It saves everyone considerable time. However, this panel recommends that there be a record of the number of white papers submitted and their fate.

The instructions to the reviewers of proposals should include a request for a final recommendation (e.g., SISGR used a verbal/numerical ranking system) that is supported by the summary statement.

Notwithstanding the prominence of BES as a funding agency for the physical sciences, for some sub-disciplines it is still important to raise the profile of BES as a potential source of research support. A higher profile would attract to BES a broader range of researchers and the disciplines they represent.

BES Program Managers should attend national and international meetings, and their practice of giving presentations about BES programs should continue (e.g., as has been done at national meetings).

(b) Monitor active project and programs

Findings:

The primary means of monitoring university grants appears to be the annual reports, including those written for renewals. The primary means of monitoring National Laboratory grants is the site visits, which are held every three years; the evaluations are thoroughly done. The reviewers' summaries are well informed, detailed, and very useful in evaluating the programs.

The principal investigator meetings are important events that provide critical information for review and provide researchers with the opportunity to meet, discuss science, and develop collaborations. The limitation of attendance primarily to principal investigators has the

advantage of leading to small, high-quality meetings, but it has the disadvantage of failing to bring into the community promising young scientists who are engaged in the projects.

Comments and Recommendations:

The panel recommends broadening the attendance at principal investigator meetings to include more young investigators, such as promising post-doctoral fellows. The selection process could reflect important contributions to on-going BES projects.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

The funded projects are consistent with the BES mission and are synergistic with projects in other BES programs. The quality of the funded work is high, and it covers a wide range of relevant topics. This work is interdisciplinary, particularly in the case of the SISGR program. The Heavy Elements Chemistry Program is as broad as can be expected given its modest size. Its portfolio is uniquely relevant to the DOE mission.

Because of the human capital needs, the Heavy Element Chemistry program may require special efforts on the educational front. This matter is of particular concern in view of the interest in expanding nuclear power generation as a carbon-free source of energy.

The panel is strongly supportive of the BES support for the excellent ACS Radiochemistry Summer School program.

It was not possible for this panel, within the time constraints of the COV meeting, to evaluate the balance of the research portfolio with respect to innovation and high-risk research.

Comments and Recommendations:

To increase the size and prominence of the Heavy Element Chemistry Program, it might be helpful combine it with the parts of the Separations and Analysis Program that deal with actinide separations. The remaining Separations and Analysis program is a strong, diverse portfolio of research topics that include the following: selective membranes, nanoporous materials, gas-phase separation (especially of CO_2 from methane), gas sequestration, liquid chromatography, photovoltaics, metal ion separations, etc. It is not clear what is envisioned as the appropriate content of the Separations and Analysis program. This very strong and diverse program might benefit from a clear description of its goals and breadth. Such a statement could lead to greater visibility and increased interest in participation in the program and thus, to a larger number of proposals.

Recognizing that is it well possible to carry out actinide research at universities, this panel recommends support for more such university projects.

The panel also recommends improved coordination and advertising of the various summer schools concerned with radiochemistry and actinide science (DHS, NE, and Office of Science).

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

Findings:

On the basis of the panel's knowledge of the fields, it has concluded that the Heavy Element Chemistry/Separations and Analysis programs support a distinguished, high-profile group of researchers. Notwithstanding the panel's very positive impression of these researchers, the panel judges that it would be useful to provide quantitative assessments / metrics of performance and suggests that they may be different for researchers at universities and National Laboratories.

Comments and Recommendation:

The panel looks forward to the implementation of the PAMS capability and the opportunity to develop quantitative metrics of the impact and outcome of the research programs (e.g., publications and citations and numbers of graduate students, numbers of supported researchers, and subsequent career paths for graduate students and post-docs).

More General Findings:

The panel judges that the DOE web pages do not provide clear, understandable descriptions of the BES research programs and grant opportunities. By "understandable" we mean accessible to people with a wide variety of scientific backgrounds. Keyword searches on Google and grants.gov do not bring up BES programs. For example, "photosynthesis," "photosynthetic systems," "photosynthesis research grants" do not lead to DOE web sites.

Comments and Recommendations:

The panel suggests that BES examine and rework as needed all of the web pages for BES research programs to provide clear, accessible, and generally understandable descriptions of the research programs and grant opportunities. Further, the panel recommends implementation of a process to determine how easily a person can find the pertinent BES web pages and grant opportunities with keyword searches in Google, grants.gov, and other sources. One might assume that the searcher would know nothing about DOE and its programs. It would also be helpful to determine how to address the deficiencies of such keyword searches. We judge that the oft-voiced criticism that DOE is an "insider" organization derives in part from its opacity, from the difficulty in finding and understanding the grant opportunities that exist there. The panel is of the view that the health and vitality of the BES research enterprise could be greatly strengthened by increasing its visibility and accessibility to more potential grant applicants via the World-Wide Web.

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

1. 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:

Excellent

Comments:

The Separations and Analysis portfolio provides significant examples of improved chemical imaging techniques that enable development and evaluation of nanometer-scale structures. These techniques have broad applicability. The portfolio also includes projects making important progress toward building of structures with nano-scale control to provide advanced separation methods. The Heavy Element Chemistry portfolio also includes projects in which exciting progress is being made in the development of methods to control actinide material structures at the nano-scale. The current research is outstanding as indicated by the quality of the publications and the comments regarding new and renewal proposals made by reviewers with excellent technical expertise.

2. 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:

Excellent

Comments:

The comments made in the immediately preceding section are equally relevant here.

3. Develop new concepts and improve existing methods for 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:

Excellent

Comments:

The evaluation is based mainly on anecdotal information, but the Panel believes that the BES programs are providing a strong basis for developing new and high-impact technologies that will find application in energy programs.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

Although the panel judges that the output of this program is of excellent quality and of high impact, the specific wording employed in this GPRA question to define "excellent" did not seem to be the best match to the portfolios the panel was asked to review. The definition alluded specifically to instrumentation for X-ray, neutron, and electron-beam scattering, which were not a part of this program. Curiously, the definition of "Good" appears to be a higher ranking than that described by “Excellent.”

Panel 7: Geosciences

I. EFFICACY AND QUALITY OF THE PROGRAM’S PROCESSES

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

Findings:

Documentation of the proposal files examined by the panels is complete and well organized. Summary statements are detailed and accurate. The files demonstrate that the number of reviews of each proposal met or exceeded the required number. The reviewers are experts in the field and provide a well-balanced diversity, both in scientific sub-disciplines and other terms. Declines were made within six months; funded proposal notifications were typically prompt, but they sometimes took up to a year if delayed by circumstances such as federal budget actions or other issues beyond the control of BES. There is excellent consistency with criteria stated in program solicitations.

Comments:

The declined proposals have shortcomings in methods, potential scientific impact, or other key characteristics (such as falling outside of the core areas). New start decisions were the most

difficult and received appropriate scrutiny through a screening process involving pre-proposal "white papers." Reviewers were not required to give an overall numerical ranking in their proposal evaluations.

The Program Manager needs an assistant (Detailee) who can commit to more than a year. He currently has ¼ time assistance and is searching for a full-time person. Qualified people are not readily available. This assistance would allow the Program Manager to devote more time to other issues including development of RFPs and travel to meetings and for site visits. Furthermore, Detailees experienced with this program provide the best pool of candidates for a successor to the current Program Manager. A Detailee would enhance continuity and institutional memory. The program relies on the long-term experience and detailed knowledge of the Manager.

The Geosciences program benefits in many ways from skilled and experienced management. The Manager has anticipated areas of national need and helped nurture investigators to address the fundamental physical and chemical principles related to these needs. A good sense of what makes for successful research is demonstrated by the program's record and the review documents. The Program Manager guides the development of the program to incorporate new scientific advances. There is a strong commitment to funding new investigators and members of underrepresented groups. Management has shown a good sense of programmatic direction and a justified willingness to take risks.

It is important for the Program Manager to travel in order to stay informed of cutting-edge research and to act as an ambassador for this program.

Recommendations:

Hire a full-time Detailee as soon as possible to maintain full program staffing and effectiveness.

Increase the travel budget to allow for attendance at key scientific conferences (national and international), site visits, and meetings to learn about new and emerging areas.

Any presentations or materials distributed at meetings and workshops regarding the program, solicitation, and the review process should be made available on the web in a timely fashion.

(b) Monitor active project and programs

Findings:

Annual principal investigator meetings in this program provide a platform for presentations of cutting-edge results. They are often topical, occur in timely and regular fashion, encourage collaborations, and include people who are not currently funded by the program and who give good feedback. Many annual progress reports are truly outstanding. Program management is readily available to principal investigators, easy to reach, and gets back to principal investigators quickly. The program is currently transitioning successfully to on-site reviews for the national laboratories.

Comments:
Consideration should be given to allow attendance at principal investigator meetings by junior scientists.

Recommendations:

The program should receive increased funding to support multiple site visits, conference attendance, and other professional travel by Program Managers.

II. EFFECT OF THE AWARD PROCESS ON PORTFOLIOS

(a) the breadth and depth of portfolio elements

Findings:

The overall quality of the science is exceptional. Research funded by this program has some of the highest impact in all of the geosciences. In the disciplines funded, this program supports some of the best research in the U.S. and the world. Funded projects are of clear importance to the DOE mission.

This program has contributed significantly to careers of junior scientists, many of whom have become internationally recognized as leaders in their fields.

Comments:

The relevance and impact of the research portfolio in geosciences far exceeds its portion of the DOE budget. This unique program is an important part of BES, with a research portfolio that complements other programs. Many of the projects would not fit with research programs elsewhere in DOE or other federal agencies. This division is a fundamental research division, and the applications to the mission of DOE are many, including, for example: CO_2 sequestration, contaminant fate and transport, nuclear waste management, extraction and remediation of fossil fuels and strategic metals, and novel nanoparticle materials.

This program also supports the development and novel applications of many new and cutting-edge analytical techniques including the following: neutron scattering, synchrotron X-ray scattering and spectroscopy, and secondary ion mass spectrometry. The program has resulted in the development of new methods of monitoring and numerical modeling of reactive transport in complex environments, including subsurface geophysical imaging methods.

The Geosciences program provides essential funding for a number of important sub-surface science areas. Many truly exceptional projects are funded that do not have another federal funding source. Much of the funded science is fundamental, with clear relevance to the mission of DOE as defined in the report "Basic Research Needs for Geosciences." This program funds interdisciplinary and inter-institutional projects, including a balance of innovative and higher-

risk projects. The long-term track record shows that these risks have paid off in terms of productivity and impact.

The depth and breadth of principal investigator backgrounds is impressive. There is a good percentage of younger investigators and documented turnover in principal investigators and in new research thrusts.

On the basis of the information examined, the panel has inferred that the Geosciences principal investigator roster is appropriately diverse. For instance, this program has supported the early research and career development of many excellent female scientists, including two who are members of the National Academy of Sciences.

The COV review would be facilitated by compiled demographic data (e.g., lists of applicants and participants from under-represented groups, ages, stages in career, students, discipline, longevity of funding, publications, and citations). The anticipated availability of such information when PAMS is implemented would likely help justify the actions and demonstrate the openness of BES and help counter the impression shared by some that the program is "closed."

Award size, scope, and duration are appropriate given current funding constraints.

Recommendations:

The early implementation of PAMS would be helpful to future COVs.

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

Findings:

Many of the principal investigators have received prestigious national and international awards.

The Geosciences program supports a high proportion of pioneering projects in areas such as the following: mineral nanoparticles, biogeochemistry, neutron scattering and synchrotron radiation studies of geologic and environmental materials and processes, simulation of multi-scale systems, and modeling of reactive transport.

Comments:

The Geosciences program has a high impact on the international research community, as evidenced by the fact that many principal investigators have received national/international awards, published in the highest-impact journals, have been frequently invited to give keynote lectures at (inter)national conferences, and have served on high-level panels and advisory boards.

The program has been managed to have a high impact on the research community.

The stature and visibility of the program depend in part on travel and communication by the Program Manager.

The impact of the Geosciences Program is enhanced by its support of graduate students, education, conferences, and publications. Numerous volumes of the influential series "Reviews in Mineralogy and Geochemistry" have been supported by this program. The articles in these books review current research, including much that was funded by BES, and achieve some of the highest impact factors in sub-surface science at a fraction of the cost charged by commercial publishers. This funding for publications, students, and post-docs strongly affects the future of critical areas of geoscience, ensuring the next generation of leaders.

This program provides the fundamental physical and chemical understanding needed to address complex subsurface phenomena critical to the DOE mission. The fundamental nature of the research enhances the ultimate depth and breadth of its impact.

With enhanced funding, there would be many opportunities to build on this research, as described in the report "Basic Research Needs for Geosciences," including investigations of the following: mineral/water interface complexity and dynamics; nano-particulate and colloid chemistry and physics; dynamic imaging of flow and transport; transport properties and in-situ characterization of fluid trapping, isolation and immobilization; fluid-induced rock deformation; and biogeochemistry in extreme subsurface environments.

Recommendations:

Continue and increase funding sufficient to support topical meetings, workshops, and review volumes.

Publicize research highlights to the national media and include more current research highlights on the web site.

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

1. 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:

Excellent

Comments:

The Geoscience program excels in providing fundamental understanding (modeling, characterization, imaging, and analysis) of mineral nano-particles that contributes to more applied research in fabrication. The geosciences lead in characterization of natural materials and

processes over a range of scales from molecular to field-scale. New understanding in areas such as interfacial processes, self-assembly, and biomineralization results from novel applications of the techniques and procedures that are being developed (including synchrotron techniques, neutron scattering, secondary ion mass-spectrometry, atomic force microscopy, and electron microscopy, including environmental TEM and SEM). Geoscientists have decades of experience with nanomaterials and colloids in the natural environment and expertise that allows science to emerge in other fields. The Geoscience program creates new knowledge and both draws knowledge from and transfers knowledge to other scientific communities, fostering synergy with programs that are central to new material development and fabrication.

2. 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:

Excellent

Comments:

The Geosciences program deals with complicated interfaces using state-of-the-art interdisciplinary approaches. Geoscientists encounter some of the most complex surfaces through study of the natural world. This program has long been at the global forefront in investigation of mineral-fluid interfaces. Many of these accomplishments are described in the 2007 report "Basic Research Needs for Geosciences."

3. Develop new concepts and improve existing methods for major energy research needs identified in the recent Basic Energy Sciences Advisory Committee "research needs" workshop reports.

Progress rating for the program under review:

Excellent

Comments:

The selection process for SISGRs is clearly in line with directions in the report "Basic Research Needs for Geosciences." Reorganization and unification of FWP support at National Laboratories has helped to set more coherent directions. Restructuring of these national laboratory programs is appropriate and being done objectively. For example, excellent progress was made by restructuring at Oak Ridge that helped focus work on basic research needs.

4. Demonstrate progress in conceiving, designing, fabricating, and using new instruments to characterize and ultimately control materials.

Progress rating for the program under review:

Excellent

Comments:

The Geoscience program has helped to support development and creative application of many important new tools for imaging and analysis, including the following: synchrotron radiation methods such as X-ray microprobe, X-ray reflection interface microscopy (XRIM), resonant anomalous X-ray scattering (RAXR) at mineral-fluid interfaces, in-situ analysis by ion beams (secondary ion mass spectrometry) that allows isotopic analysis of nano- to pico-gram samples with unprecedented accuracy, and SANS/USANS/QENS (small-angle neutron scattering, ultra-small-angle scattering, and quasi-elastic neutron scattering).