Update on the Upcoming COV of the BES Chemical Sciences, Geosciences, & Biosciences Division

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Office of Basic Energy Sciences
Office of Science
U.S. Department of Energy

BESAC Meeting, February 21, 2008

Outline

- **2008 COV (FY2005-2007)**
  - Charge
  - Organization and membership
- **2005 COV (FY2002-2004)**
  - Recommendations and actions
- **Changes in the division**
  - Organizational, staffing, and program changes since last COV
- **COV preparatory work**
  - November 7, 2007 meeting between chair and division, COV website, etc.

2008 Committee of Visitors Review of the BES Chemical Sciences, Geosciences, and Biosciences Division

April 23-25, 2008

DOE Germantown, MD

All BESAC members are welcome!

Charge letter

UNIVERSITY OF CALIFORNIA, IRVINE

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October 4, 2007

Professor Geraldine Richmond
Richard M. and Patricia H. Noyes Professor
Department of Chemistry
212 Willamette Hall
1253 University of Oregon
Eugene, OR 97403-1253

Dear Professor Richmond:

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 2005, 2006, and 2007. 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
(3) Photochemistry and Radiation Research
(4) Catalysis and Chemical Transformations
(5) Separations and Analyses
(6) Heavy Element Chemistry
(7) Chemical Engineering and Chemical Energy
(8) Geosciences Research
(9) Energy 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 23-25, 2008 at the BES/DOE Germantown location at 19901 Germantown Road, Germantown, Maryland 20874-1290. A presentation to BESAC is requested at its Summer 2008 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 Office of Management and Budget (OMB) evaluation of Basic Energy Sciences progress toward the long-term goals specified in the OMB Program Assessment Rating Tool (PART, attached). Each of the nine components (or sub-components, if appropriate) of the Chemical Sciences, Geosciences, and Biosciences Division should be evaluated against each of the four PART 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 OMB 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 Karen Talamini, Office of Basic Energy Sciences at 301-903-4563 or by e-mail at karen.talamini@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

Attachment

cc: P. Dehmer
E. Rohlfing
K. Talamini
D. Marceau

Geri Richmond is COV chair

COV Charge

- **The panel should assess the operations of the Division's programs in FY2005, 2006, and 2007 in these areas:**

  AMO Sciences, Chemical Physics, Photochemistry & Radiation Research, Catalysis & Chemical Transformations, Separations and Analyses, Heavy Element Chemistry, Chemical Engineering and Chemical Energy, Geosciences, and Energy Biosciences

- **The panel may examine any files during the review period for both DOE lab and university projects (subject to COI constraints).**

- **Two major review criteria:**

  1) **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.**

- **The COV panel is asked to provide input on the BES OMB Performance Assessment Rating Tool (PART) long-term goals.**

2008 COV Organization and Membership

- **Chair: Geri Richmond,** University of Oregon**

- **Panel 1: AMO Sciences/Gas-Phase Chemical Physics**

  Panel Lead: Carl Lineberger,** University of Colorado (2002 COV)

  Members: Tom Gallagher, University of Virginia
  Anthony Johnson,** University of Maryland
  Kate Kirby,* Harvard-Smithsonian CFA
  Arthur Suits, Wayne St. University
  Sotiris Xantheas, Pacific Northwest National Lab

- **Panel 2: Photochemistry/Condensed Phase Chemical Physics**

  Panel Lead: Peter Rossky, University of Texas (2005 COV)

  Members: Luis Echegoyen, NSF & Clemson University
  Etsuko Fujita, Brookhaven National Laboratory
  Devens Gust, Arizona State University
  Sharon Hammes-Schiffer,* Pennsylvania State University
  Thom Orlando, Georgia Tech

- **Panel 3: Catalysis**

  Panel Lead: Bruce Gates,* UC Davis

  Members: Cynthia Friend, Harvard University (2005 COV)
  Horia Metiu, UC Santa Barbara
  Umit Ozkan, Ohio State University
  Simon Bare,* UOP LLC
  D. Michael Heinekey, University of Washington

Funded by CSGB Division
*Current BESAC member
**Past BESAC member

2008 COV Organization and Membership

- **Panel 4: Heavy Element Chemistry/Separations & Analyses**

  Panel Lead: Carol Burns, Los Alamos National Laboratory (2002 COV)

  Members: Bruce Chase, Dupont
  Sue Clark,* Washington State University (2005 COV)
  William Evans, UC Irvine
  Michael Heaven, Emory University
  Robert Hettich, Oak Ridge National Lab

- **Panel 5: Geosciences**

  Panel Lead: Ed Stolper, Cal Tech

  Members: Bob Bodnar, Virginia Tech
  Randy Cygan, Sandia National Laboratories
  Dianne Newman, MIT
  Lars Stixrude, University College London
  Jim Tyburczy, Arizona St. University

- **Panel 6: Biosciences**

  Panel Lead: Elizabetth Gantt, University of Maryland

  Members: Robert Blankenship, Washington University
  John Richards,* Cal Tech (2005 COV)
  John Shanklin, Brookhaven National Laboratory (2005 COV)
  Judy St. John, USDA

Funded by CSGB Division

*Current BESAC member

**Past BESAC member

2008 COV Membership Summary

- **36 total members of the COV:**

16 are currently funded by BES/CSGB
20 are not currently funded by BES/CSGB

25 are men
11 are women

27 are from academia
6 are from DOE labs (but 2 academics have previous lab experience)
2 are from industry
1 is from another Federal agency (not counting Luis Echegoyen)

13 are from the East
10 are from the Midwest
13 are from the West

7 have served on CSGB COVs in 2002 or 2005

9 are current or previous BESAC members

2005 COV recommendations and actions

- **Program management database**

  Recommendation: Create a BES database for peer review/program management.

  Actions: Modest improvements in SC database (IMSC); more effective use of IMSC.

- **Improved proposal solicitation**

  Recommendation: Use "Dear Colleague" mailings to community in addition to normal postings on SC website.

  Action: Department chair "Dear Colleague" lists developed and used for Chemical Imaging (FY2006) and SEU (FY2007) solicitations.

- **Long-term support for basic research & young investigator program**

  Recommendation: Continue "tradition" of long term support, but also consider implementing a young investigator program.

  Actions: A significant young investigator program is not feasible under current budget constraints. Award for BES PECASE winners codified ($50k/yr for 5 years). BES solicitations have allowed more young investigators to be funded.

- **Diversity**

  Recommendation: BES should collect demographic data on gender, race, and career-stage and efforts should be made to ensure a diverse work force.

  Actions: SC-wide demographic data collection system "in progress;" CSGB co-sponsored gender and URM equity in chemistry workshops with NSF and NIH.

2005 COV recommendations and actions

- **Re-evaluate and re-focus Energy Biosciences program – integrate it within the Division**

  Recommendation: New program management should re-evaluate and re-focus program on BES missions; program should be better integrated with division

  Action: Under new program leadership (Rich Greene), program has been redefined into two components – Solar Photochemistry and Physical Biosciences. Significant shifts in the portfolio are underway. Team structure changed to foster improved integration (see following).

- **Program management staff**

  Recommendation: division be given at least three new program manager positions

  Action: BES staffing budget in FY2008 includes 3 new program manager positions in CSGB (see following).

- **Portfolio prioritization**

  Recommendation: In light of flat funding, prioritize the portfolio in order to continue supporting areas critical to DOE mission at appropriate level.

  Action: significant prioritization accomplished – see following.

Changes in CSGB division

- **Organizational changes**

  FY2007: Chemical Physics program split into two parts: Gas-Phase Chemical Physics (combustion related) and Condensed Phase & Interfacial Molecular Science (CPIMS)

  FY2008: Created the new Photo- and Biochemistry Team from the Energy Biosciences program plus the Solar Photochemistry program (from Fundamental Interactions); associated modest program name changes

- **Significant program changes (portfolio optimization)**

  FY2006 – 2008: Phase out of the Chemical Energy & Chemical Engineering Program

  - Motivated by budgetary pressure and a lack of coherence in the program
  - A few research projects moved to Catalysis Science; most funding reprogrammed

  FY2005 – 2007: Investment in ultrafast chemical science, principally in AMOS program (UXSL at LBNL; PULSE at SLAC)

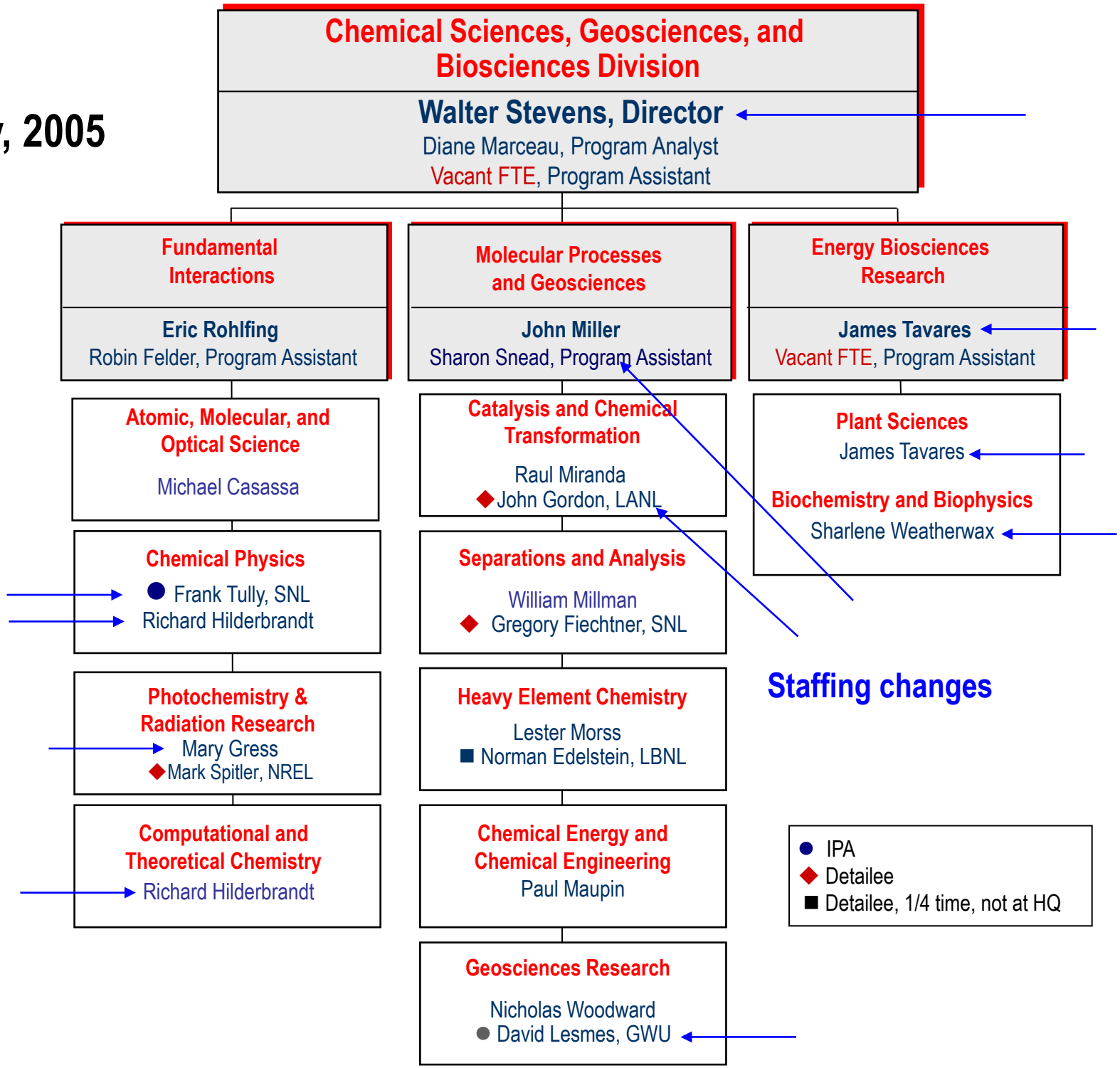
  FY2006: Investment in chemical imaging across division

- **Staffing**

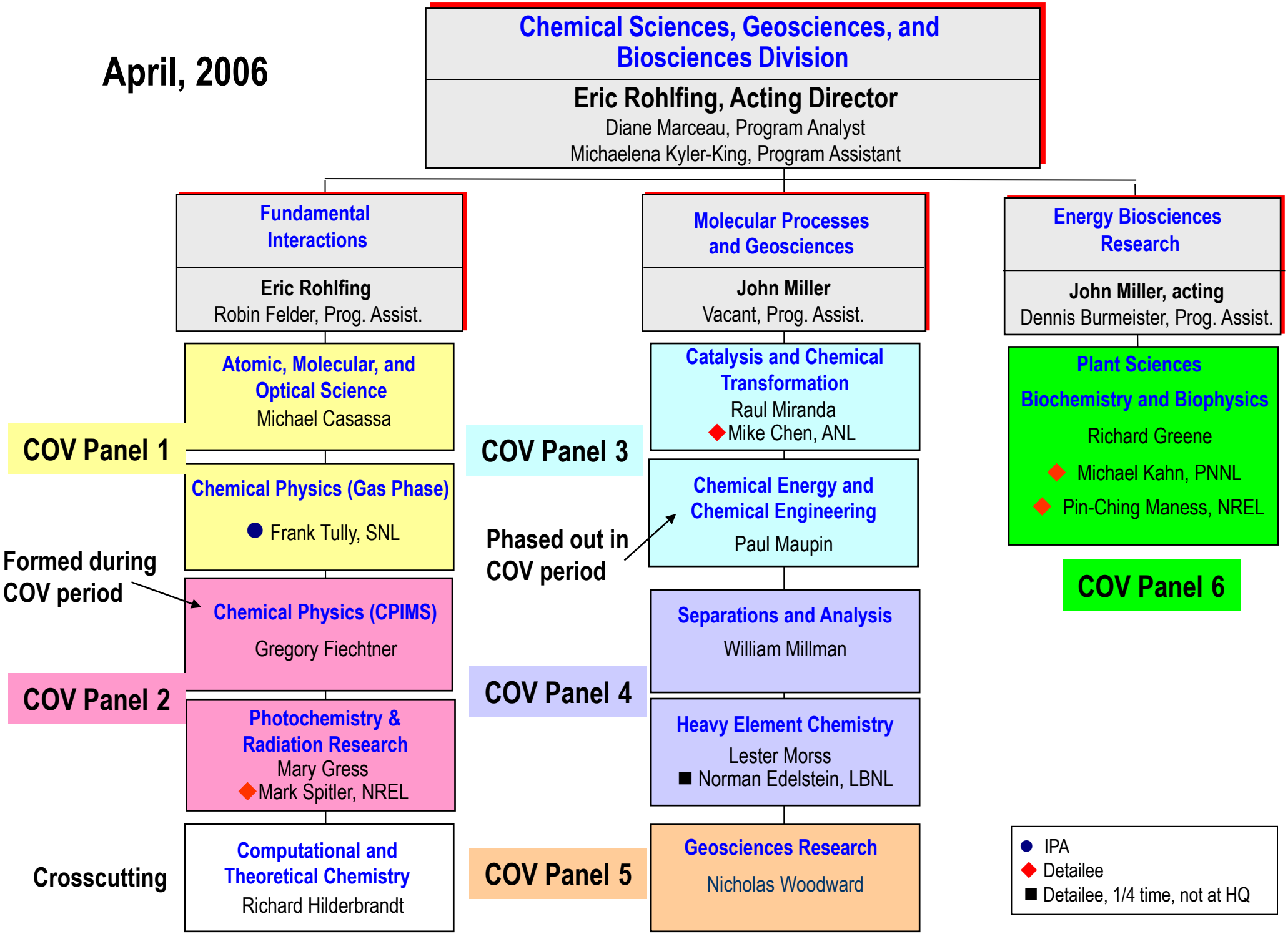
  Significant changes in division staff since the last COV

  Significant (but transient!) understaffing during upcoming COV

February, 2005



April, 2006


Chemical Sciences, Geosciences, and Biosciences Division
Eric Rohlfing, Acting Director
Diane Marceau, Program Analyst
Michaelena Kyler-King, Program Assistant
Fundamental Interactions
Eric Rohlfing
Robin Felder, Prog. Assist.
Molecular Processes and Geosciences
John Miller
Vacant, Prog. Assist.
Energy Biosciences Research
John Miller, acting
Dennis Burmeister, Prog. Assist.
Atomic, Molecular, and Optical Science
Michael Casassa
COV Panel 1
Chemical Physics (Gas Phase)
● Frank Tully, SNL
Formed during COV period
Chemical Physics (CPIMS)
Gregory Fiechtner
COV Panel 2
Photochemistry & Radiation Research
Mary Gress
◆ Mark Spitler, NREL
Crosscutting
Computational and Theoretical Chemistry
Richard Hilderbrandt
Catalysis and Chemical Transformation
Raul Miranda
◆ Mike Chen, ANL
COV Panel 3
Phased out in COV period
Chemical Energy and Chemical Engineering
Paul Maupin
Separations and Analysis
William Millman
COV Panel 4
Heavy Element Chemistry
Lester Morss
■ Norman Edelstein, LBNL
COV Panel 5
Geosciences Research
Nicholas Woodward
Plant Sciences
Biochemistry and Biophysics
Richard Greene
◆ Michael Kahn, PNNL
◆ Pin-Ching Maness, NREL
COV Panel 6
● IPA
◆ Detailee
■ Detailee, 1/4 time, not at HQ

April, 2008?

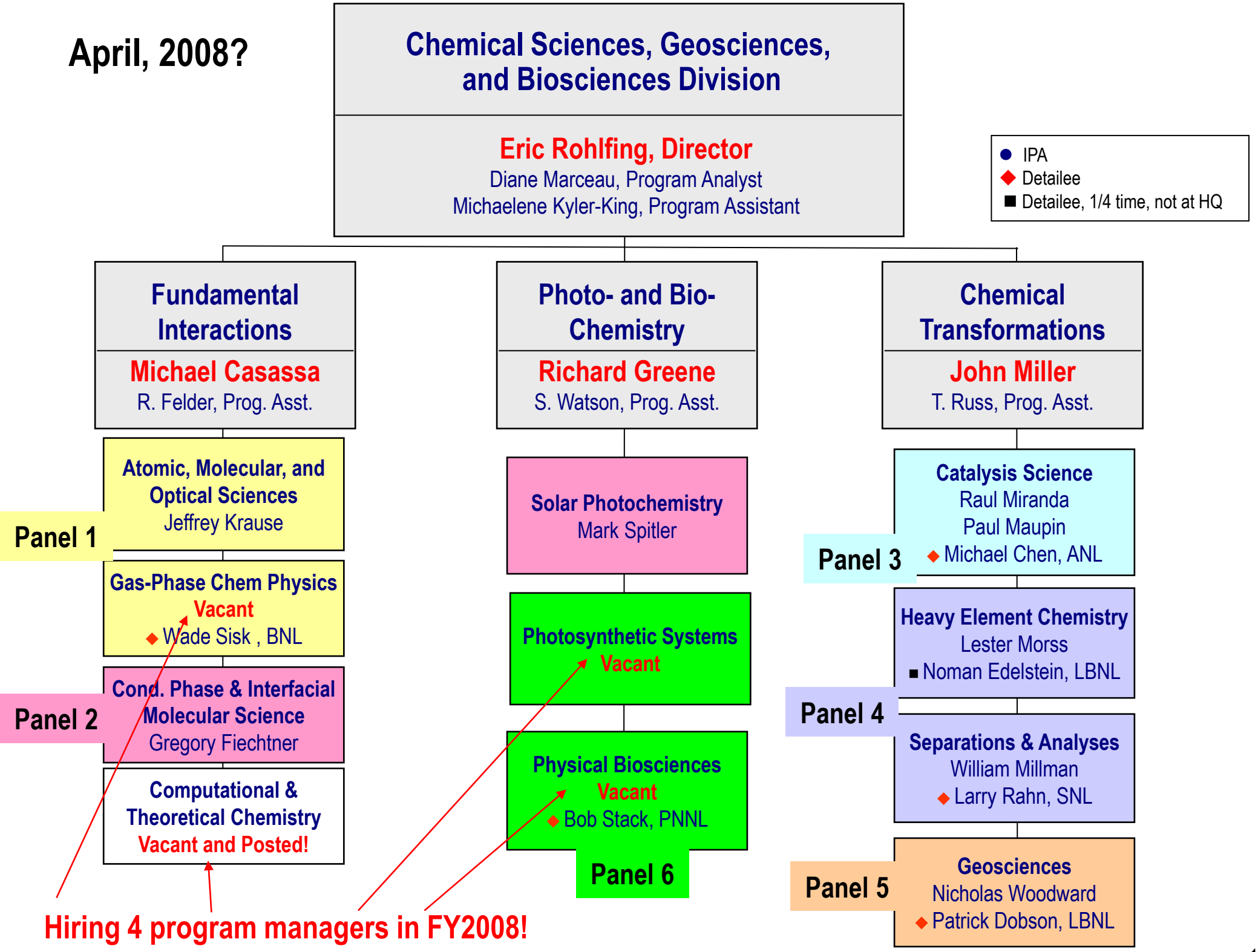

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Photo- and Bio-Chemistry
Richard Greene
S. Watson, Prog. Asst.
Chemical Transformations
John Miller
T. Russ, Prog. Asst.
Atomic, Molecular, and Optical Sciences
Jeffrey Krause
Panel 1
Gas-Phase Chem Physics
Vacant
Wade Sisk , BNL
Cond. Phase & Interfacial Molecular Science
Gregory Fiechtner
Panel 2
Computational & Theoretical Chemistry
Vacant and Posted!
Solar Photochemistry
Mark Spitler
Photosynthetic Systems
Vacant
Physical Biosciences
Vacant
Bob Stack, PNNL
Panel 6
Catalysis Science
Raul Miranda
Paul Maupin
Michael Chen, ANL
Panel 3
Heavy Element Chemistry
Lester Morss
Noman Edelstein, LBNL
Panel 4
Separations & Analyses
William Millman
Larry Rahn, SNL
Geosciences
Nicholas Woodward
Patrick Dobson, LBNL
Panel 5
Hiring 4 program managers in FY2008!

Program manager for computational and theoretical chemistry

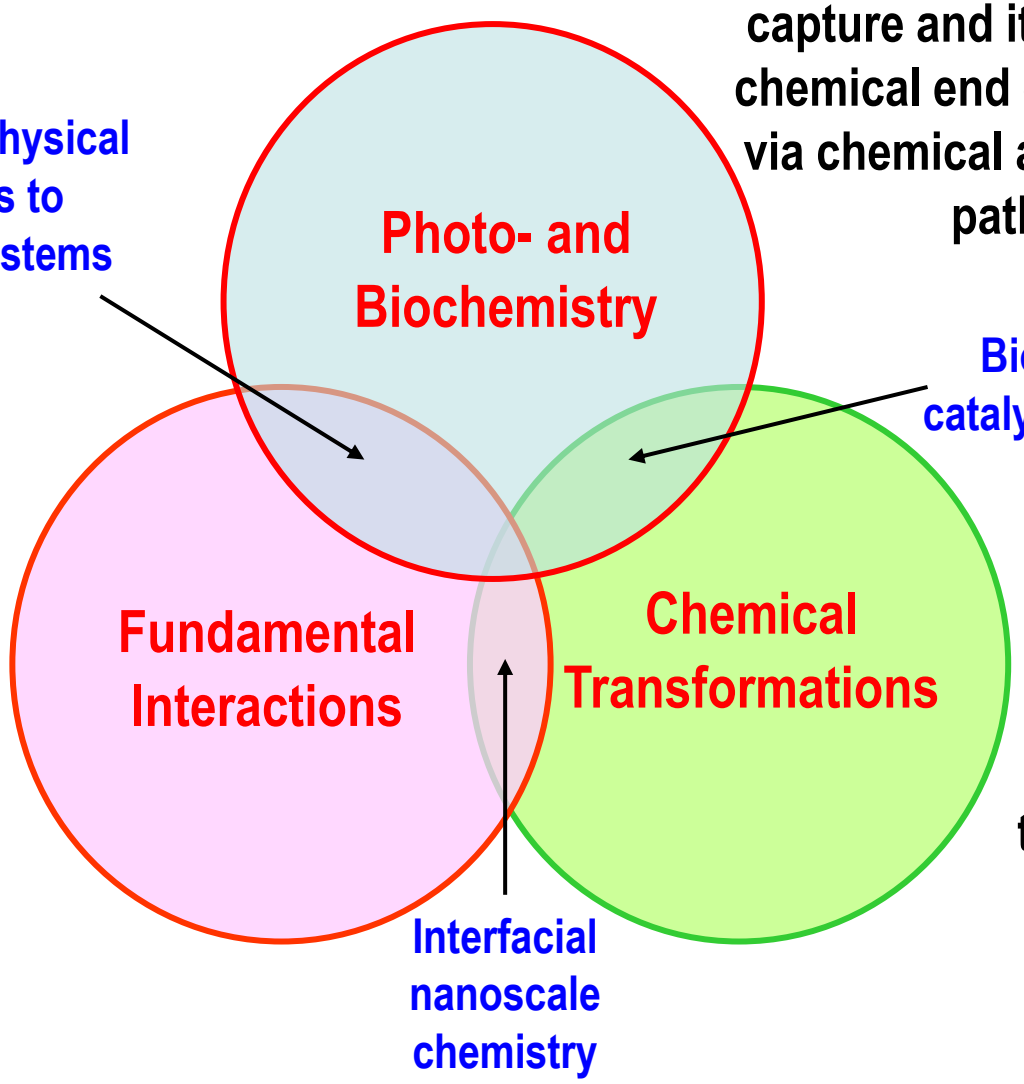
Dick Hilderbrandt retired after 21 years of Federal service on December 31, 2007

Job Opportunity: Program Manager for Computational and Theoretical Chemistry

The Office of Basic Energy Sciences (http://www.sc.doe.gov/bes/bes.html), Office of Science, US Department of Energy, is seeking qualified applicants for a career federal position managing the Computational and Theoretical Chemistry Program, funding mission-oriented basic science at universities and national laboratories. The program encompasses a broad range of computational and theoretical approaches to scientific discovery in areas of interest to DOE. The research includes understanding and predicting the properties and chemical behavior of molecular systems and complexes in the gas phase, in solution, at interfaces, and in biological systems. It emphasizes development of new theories, methods and algorithms for applying theoretical and computational science and simulation to understanding chemical behavior and molecular properties in a wide range of environments, including new opportunities and challenges in complex systems, nanoscale materials, solar energy utilization, and ultrafast science. The program manager also assists in the allocation of computer resources at Office of Science high-performance computing facilities.

The announcement and on-line application instructions can be found via the BES website: http://www.sc.doe.gov/bes/BESjobs.html or directly at USA Jobs: http://jobsearch.usajobs.gov/ftva.asp?seeker=1&JobID=68052643 . Applications must be submitted by 11 pm on **April 21**, **2008.**

CSGB Team Structure



Molecular mechanisms of light capture and its conversion to chemical end electrical energy via chemical and biochemical pathways

Application of physical science tools to biochemical systems

Biomimetic catalytic systems

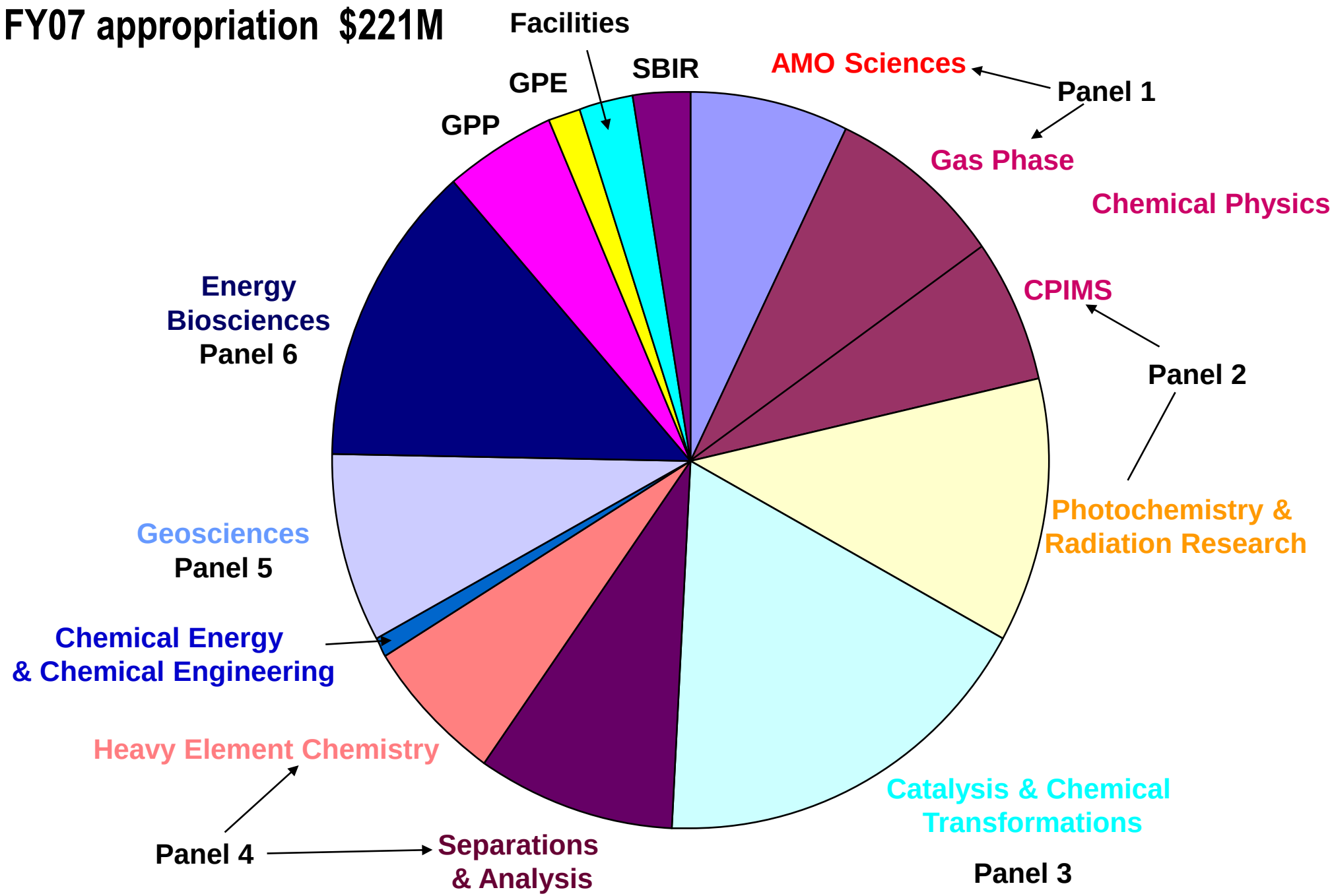
Structural and dynamical studies of atoms, molecules, and nanostructures; description of their interactions with external stimuli (photons, electrons) at full quantum detail

Characterization, control, and optimization of chemical transformations, from catalysis to geochemistry

Interfacial nanoscale chemistry

- Division-wide themes: chemical imaging; ultrafast chemical sciences; nanoscale science; catalysis science; theory, modeling, & simulation; synthesis

CSGB Budget Distribution



Solicitations with impact during COV period

- **Notice 04-20, *Basic Research for the Hydrogen Fuel Initiative***
  - Published in FY2004; awards made in FY2005
  - Large, BES wide initiative that provided ~$21M in new funds across BES; supplemented by ~$3M in FY2006
  - ~38 awards assigned to several programs in CSGB; under renewal review in FY2008 as an integrated program across BES
- **Notice 05-30, *Basic Research for Chemical Imaging***
  - Published in FY2005; awards made in FY2006
  - Modest, CSGB only initiative that reprogrammed ~$3M within CSGB
  - ~17 awards in nearly every program in the division
- **Notice 06-15, *Basic Research for Solar Energy Utilization***
  - Published in FY2006; 27 awards made across BES with modest funding (~$8M) in FY2007
  - 14 awards in CSGB in Solar Photochemistry and Biosciences programs
- **Notice 06-17, *Basic Research for the Hydrogen Fuel Initiative***
  - Published in FY2006; 13 awards made across BES with modest funding (~$4M) in FY2007
  - 6 awards in CSGB in Catalysis Science program

COV preparatory work

- **November 7 meeting between Geri Richmond and Division**
  - **Opportunity for chair to meet with the entire division to understand our structure and programs**

    Geri used this successfully as chair of the 2007 COV for NSF Chemistry Division

    She felt it important to understand the differences between NSF and BES

  - **Full (almost) day visit**

    Divisional overview presentation

    Presentation on COV information

    Informal discussions between Geri and program managers/team leads in each program

- **Next steps for COV**

  Completion of the membership drive – finished in December, 2007

  Plans for COV website – now operational and will be updated with new information

  Additional teleconferences with chair and with chair/panel leads before COV

Information for the 2008 COV

- **Prior to COV – via password-protected website (ORISE)**
  - COV roster (soon to be updated for second read assignments)
  - Charge letter
  - Reports from 2002 and 2005 COVs (links to BES website)
  - Review procedures (links to BES website)
  - Core research activity descriptions (links to BES website, with updated versions for COV)
  - Published solicitations during COV period (links to SC Grants website)
  - Logistical details (agenda, travel, lodging, etc.)
- **During COV**
  - BES and Division overview presentation
  - Topical overviews by team leads – topics TBD, but probably solicitations, lab reviews, etc.
  - Program overview presentations
  - Spreadsheet for each program showing every project (university and lab) that was active during three-year review period
  - Spreadsheet showing all CSGB reviewers over review period
  - Selection of university and lab review files (new awards, renewals, declinations) plus access to all files (constrained by COI)
  - COV report template (including OMB PART assessments)

2008 COV website