National Science Foundation
Division of Chemistry December 2012 – Issue 19

Inside the Issue

Letter from the Division Director

Matthew Platz

Greetings,

It has been my privilege to serve as Director of the Division of Chemistry since September 2010. It is a time of reflection as I now prepare to rotate out of the Division Director's chair and pass the baton to Dr. Jackie Gervay-Hague, at the end of 2012. Accordingly, this will be my last newsletter as Division Director, and so I will use this space to give thanks, and to consider some areas in which we, as chemists, as a community, might set our sights. I believe there are numerous grand challenges facing civilization that can only be met with the discovery of new chemistry. Thus, it is important for us in the Foundation and in the Academy to re-imagine our research and teaching programs so that we are able to bring fundamental chemical insight to bear on some of the biggest problems facing humanity.

But first, it is my pleasure to acknowledge the contributions of our hard-working administrative and technical staff. It has been both inspiring and fun to serve with my colleagues here at NSF, and I thank them most sincerely for their expertise, professionalism, and collegiality. As I have mentioned before, every 10-15 years, the number of proposals the division receives doubles, but the number of NSF personnel that service your proposals stays the same. The staff has responded magnificently to this challenge and I am constantly impressed by their commitment to our mission. Long nights and weekends, reminiscent of assistant professor days, are the norm in Arlington. The program officers understand the consequences of their recommendations on Principal Investigators (PIs). Thus, they constantly look for ways to acquire co-funding to maximize the number of funded proposals, and agonize over the hundreds of worthy projects that we must decline every year. I hope that the move to one submission window will stabilize the number of submissions and set our work on the following cycle submit in the autumn, review in the winter, and funding decisions in the late spring/summer. Speaking of the review process, we are in a tight fiscal climate, and it is likely that the number of traditional panels will decrease and the number of virtual panels will increase. I also want to take this opportunity to thank you, the community, for being a critical component of the review process. We are aware that some of the very busiest scientists are among the most diligent, punctual, and thorough reviewers. Given the enormous "proposal pressure" generated by chemists seeking support to push back the frontiers of knowledge, your willingness to help referee the process, and give invaluable advice to the Division is greatly appreciated.

In my time at the NSF, and throughout my career, I have interacted with chemists with different motivations and chemists can and should be free to move along this continuum throughout their careers. Furthermore, it is the nature of chemistry that every new discovery in our field has potential applications. A perfect example is research on dihydrogen, the smallest and arguably the most "fundamental" molecule, which has enormous potential as a carbon-free fuel of the future. Every branch of science, including chemistry, can point with pride to examples of curiosity-driven research leading to practical applications that benefit

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humanity. But like other disciplines, I believe that the history of chemistry is full of examples of application-motivated research leading to emergence of new fields and new theory. One hundred years ago, a looming food shortage served as the impetus for Haber and Bosch to develop a man-made version of nitrogen fixation: namely, the metal-catalyzed reaction of nitrogen and hydrogen that bears their names. The product of their use-inspired research, ammonia, currently feeds over one third of the planet. Perhaps, in hindsight, one can see that this use-inspired research gave rise to the curiosity-driven fields of high pressure gas phase chemistry and gas/metal interfacial chemistry.

In the 21st century, meeting humanity's increasing demand for food, water and energy will be one of the greatest challenges facing civilization and one that will surely occupy the thoughts of world leaders. Defining the constraints associated with the food/water/energy nexus, and optimizing this complex function of interdependent variables will require the discovery of new chemistry. I sincerely hope that chemists vigorously accept this challenge and that chemistry becomes the "go-to" science for solving this and other pressing problems. The younger generation is full of creative individuals who want to build a sustainable world. It is up to us to convince these idealistic students, by word and example, that research in chemistry, around great global problems, is the way to realize their personal and professional dreams. Chemistry and chemists have simply never been more important to humanity. Spread the word.

Best wishes for continued success,
Matt Platz, Division Director
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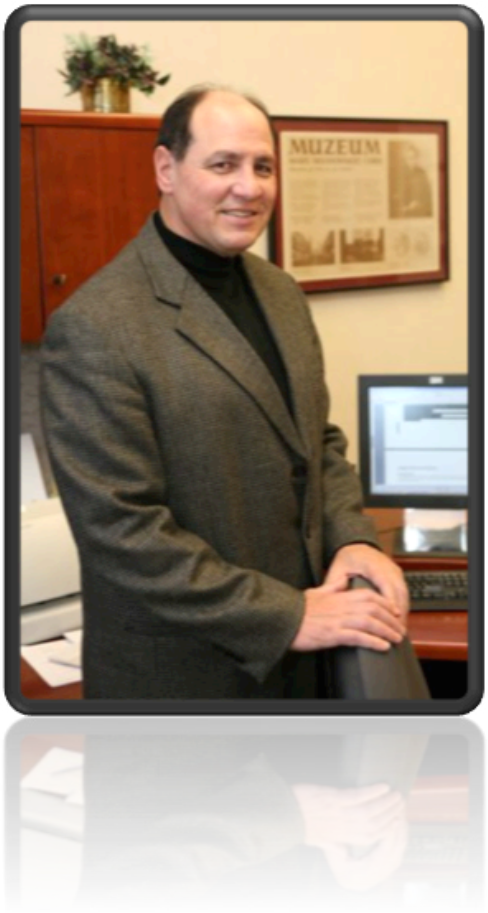

Greetings from the CHE Deputy Division Director

Tanja Pietraß

In March of 2012, I formally became the Deputy Division Director (DDD) in the Division of Chemistry. This position was previously held by Dr. Janice Hicks (who is now the DDD Division of Materials Research at NSF). Since Janice's departure, the role was temporarily filled first by Dr. Kathy Covert and then by myself. I would like to take this opportunity to thank Kathy for her service to the Division as well as for her help, support, and advice during my transition from Program Officer to DDD. Her profound knowledge of the Foundation and institutional memory are invaluable assets for the Division.

The role of the DDD is to serve as a back-up for the Division Director during his/her absences, to manage the internal operations of the Division (e.g. staffing, business processes, budget), to serve as the Conflicts Officer for the Division, and to support the Division Director and the Office of the Assistant Director in developing strategic priorities and in responding to requests from the Office of Management and Budget.

I will continue to maintain oversight of current awards made during my time as Program Director in the Experimental Physical Chemistry, Chemical Structure, Dynamics and Mechanisms, Chemical Management and Imaging, and Academic Research Infrastructure programs. However, there are certain actions that I can no longer perform (such as managing supplement requests), which will be handled by my colleagues in the respective programs.

I greatly enjoy my new position and am looking forward to working with you in the future. I hope to provide continuity in our service to the community as Matt rotates out of his position, and our new Division Director comes on board.

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Data Rising

Sharon Neal

Even if you didn't see the February New York Times Review article by Steve Lohr or news coverage of the White House's "Big Data Rollout" highlighting new and existing federal programs in March, you probably know that "Big Data" is a big story. Under the umbrella of NSF's Cyberinfrastructure Framework for 21st Century Science and Engineering (CIF21), the Foundation is ramping up a number of programs focused on developing a "comprehensive, integrated, sustainable, and secure cyberinfrastructure (CI) to accelerate research and education and new functional capabilities in computational and data-intensive science and engineering."

NSF has a number of programs designed to support the development of infrastructure to improve the utility of scientific data and research utilizing scientific data in new ways. This synopsis will focus on two programs and one activity that may be of interest to our communities:

Core Techniques and Technologies for Advancing Big Data Science & Engineering (BIGDATA, NSF 12-499)

Data Infrastructure Building Blocks (DIBBs, NSF 12-557)

DataWay Charrette (http://www.nsf.gov/mps/dataway/dataway.jsp)

For the purposes of this discussion, "big data" is defined in the NSF 12-499 solicitation as "large, diverse, complex, longitudinal, and/or distributed data sets generated from instruments, sensors, Internet transactions, email, video, click streams, and/or all other digital sources available today and in the future."

The BIGDATA solicitation is a Foundation-wide initiative coordinated with multiple agencies that seeks to advance core scientific and technological means of managing, analyzing, visualizing, and extracting useful information from large, diverse, distributed and heterogeneous data sets. The window for proposal submission for this year ended on July 11, 2012, so this year's reviewing cycle will have started by the time you're reading this, but this initiative is expected to continue.

The DIBBs solicitation is a response to the realization that "digital data are not only the output of research, but their analysis provide input to new hypotheses, enable new scientific insights, drive innovation, and inform education." The program is managed by the Office of Cyberinfrastructure and seeks to support scientific communities as they conceptualize, develop, implement, and share new methods, management structures, and technologies to store and manage the diversity, size, and complexity of their current and future data sets and data streams. Full proposals for the conceptualization track were due on July 26, 2012, and proposals for the implementation and interoperability track were due on August 30, 2012.

The DataWay Charrette is an opportunity for scientists and engineers in all disciplines to help the Foundation and other agencies plan the development of data management infrastructures integrated across the sciences and engineering with a focus on providing access and knowledge extraction to "the long tail" of heterogeneous, diverse data collected from the various sources of digital data, including sensors, instruments, simulations, transactions and data streams, regardless of the scale of the constituent data elements, the number of investigators collaborating on their collection, or the investigators' discipline. Since chemists develop and use so many different types of sensors, instruments, and simulations, the chemical community can play a unique role in this initiative and identify opportunities to expand and grow in new directions as a result of its participation.

NSF has a long history of supporting computational chemistry, and the new and existing initiatives to develop of data infrastructure and data intensive science will expand the Foundation's role in supporting existing and emerging types of digital chemical science.

New: Proposal & Award Policies & Procedures Guide (PAPPG)

Renee Wilkerson

A revised version of the NSF Proposal & Award Policies & Procedures Guide (PAPPG), NSF 13-1, was issued on October 4, 2012 and is effective for proposals submitted, or due, on or after January 14, 2013. Please be advised that the guidelines contained in NSF 13-1 apply to proposals submitted in response to this funding opportunity. Proposers who opt to submit prior to January 14, 2013, must also follow the guidelines contained in NSF 13-1.

Please be aware that significant changes have been made to the PAPPG to implement revised merit review criteria based on the National Science Board (NSB) report, National Science Foundation's Merit Review Criteria: Review and Revisions. While the two merit review criteria remain unchanged (Intellectual Merit and Broader Impacts), guidance has been provided to clarify and improve the function of the criteria. Changes will affect the project summary and project description sections of proposals. Annual and final reports also will be affected.

A by-chapter summary of this and other significant changes is provided at the beginning of both the Grant Proposal Guide and the Award & Administration Guide.

Staff Changes in the Division of Chemistry

Debbie Jones

The Division would like to thank Dr. Carina Barth for her service over the last year. Also, Ms. Renee Wilkerson is on a six month detail at the Office of Management and Budget (OMB), Office of Federal Financial Management. The Division of Chemistry wishes them both continued success.

The Division welcomes the following new staff members: Dr. Carol Bessel, Dr. Frank Wodarczyk, and Ms. Margaret Anne Wampamba. Dr. Carol Bessel is returning to the Division after working as a Program Manager at the Department of Energy, in the Chemical Sciences, Geosciences and Biosciences Division of Basic Energy Sciences. Dr. Bessel will be working in the Chemical Catalysis (CAT) Program. Dr. Frank Wodarczyk is a retired Program Officer from the Division of Chemistry and will be returning on a part-time basis to work with the Chemical Catalysis (CAT) and Sustainable Energy Pathways (SEP) Programs. Ms. Margaret-Anne Wampamba comes from the Office of the Assistant Director in the Directorate of Mathematical and Physical Sciences (MPS) and will serve as a Program Specialist. Additionally, we would also like to congratulate Ms. Kimberly Noble on her promotion to a Program Specialist.

FY2013 Division of Chemistry Committee of Visitors

Renee Wilkerson and Tanja Pietraß

Every NSF division, as well as select programs, undergoes a regular performance assessment by an external Committee of Visitors (COV). The Division of Chemistry (CHE) was most recently assessed in May 2010 by a 32-member committee chaired by Professor Cynthia Burrows from the University of Utah. CHE will host its next COV in 2013.

COV members should represent the entire chemistry research community, and therefore include members who have received awards, as well as those whose proposals have been declined. The members represented mirror the entire spectrum of geographic and demographic diversity as well as types of chemistry research institutions in the U.S.

This is a committee that provides critical community oversight to the Division's operations. Their findings are reviewed by the Office of Management and Budget (OMB) and the Office of Science & Technology Policy (OSTP) and may be used in policy and budget decisions that affect the Division, and by extension, the entire chemistry community. The COV reports to the Mathematical and Physical Sciences Directorate Advisory Committee (MPSAC). During the approximately three day visit, COV members are provided with a randomly selected set of proposals and reviews that fall into one of three groups: highly competitive, borderline, or non-competitive.

COV members have access to the detailed documentation and reasoning behind the declination and award recommendations. In addition, committee members are given access to all proposal recommendations from the previous three years within conflict-of-interest rules, as well as proposal actions selected for their original packages. A questionnaire is provided to help the COV members evaluate portfolio balance, quality of decisions, and procedure. This process provides insight into the rationale behind the Division's recommendations to the COV members.

Should you be invited to serve on the upcoming COV for CHE, please give it your serious consideration, since your selection responds to a stringent set of criteria which makes you uniquely suited for the task.

Recent Directorate for Mathematical and Physical Sciences Committee of Visitors' Reports and Division responses are available at: http://www.nsf.gov/mps/advisory/cov.jsp

Laboratory Safety Workshop Report

Ty Mitchell

A groundbreaking workshop co-sponsored by the Division of Chemistry at the National Science Foundation (NSF) was held on March 15-16, 2012. The inaugural "University of California (UC) Center for Laboratory Safety Workshop" was held at the National Academy of Sciences' Beckman Center in Irvine, California. This Center was established in 2011, a first-of-its-kind laboratory safety center to study the effectiveness of lab safety programs. The inaugural workshop was designed to create a context for future health and safety studies, to develop best practices nationwide, and to provide subject matter for both national and international colloquia. The goal of the meeting was to develop priorities and topics for funding research on laboratory safety.

The workshop consisted of a diverse group of 71 researchers, students, and health and safety professionals from government, academia, and the private sector. The group was charged with establishing research priorities and criteria to empirically study laboratory safety. The workshop began with a panel discussion on the challenges and opportunities that impact academic laboratory safety. During the breakout sessions, the workgroups brainstormed problems, solutions and research plans, addressing topics such as safety Culture, Laboratory Design, Safety and Compliance Strategies, and Chemical and other Hazard Identification and Assessment. Research priorities were generated from these topics to meet the ultimate goal of translating research outcomes into evidence-based best practices in the laboratory.

This was a timely and well-planned workshop, because laboratory safety and laboratory safety training has always been a topic of interest to researchers, and has received increased attention as evidenced by recent articles on Laboratory Safety in the C&EN News and Science magazines.

The Center is working on the following initiatives, which will be completed this summer:

- Preparation of workshop proceedings and research priorities for publication and widespread dissemination;
- Development of "Request for Proposals" for workshop-generated research ideas (Application Deadline: August 2, 2013);
- Expansion of Center website to provide links to articles, useful tools, and other materials regarding laboratory safety;
- Awarding of seed funding for demonstration projects based on research topics identified at the workshop; and
- Hiring of a Research Project Manager to oversee laboratory safety research, develop and translate research into applied best practices, and facilitate the implementation and optimization of laboratory safety practices.

As a result of the Workshop, the following actions are recommended for research laboratories and researchers: (1) the development of a Chemical Hygiene Plan (see links below); and (2) participation in the laboratory safety survey that was designed and circulated by the UC Center for Laboratory Safety, Nature Publishing Group and BioRAFT. The research communities at institutions are urged to actively participate in the survey and to request that their Research Offices send the link to the survey (see below) directly to researchers at their institutions. It is hoped that the data collected in the survey will ultimately lead to data-driven improvements in laboratory safety.

Laboratory Survey
http://web.princeton.edu/sites/ehs/labsafetymanual/TOC.htm
UCLA Chemical Hygiene Plan
http://map.ais.ucla.edu/go/1002909
Princeton University Chemical Hygiene Plan

CHE at the Philadelphia ACS Meeting

Renee Wilkerson

All American Chemical Society (ACS) meeting attendees were invited to join the National Science Foundation Division of Chemistry and representatives from other federal agencies for "Federal Funders Town Hall and Speed Coaching Meeting" at the National Meeting and Exposition of the ACS in Philadelphia, Pennsylvania, Monday, August 20, 2012 in the Pennsylvania Convention Center. This outreach meeting was a partnership between the Division of Chemistry at NSF, the Chemical Sciences, Geosciences, and Biosciences Division in the Department of Energy's Office of Basic Energy Sciences, and the Division of Pharmacology, Physiology, and Biological Chemistry in the National Institutes of Health's National Institute of General Medical Sciences. Federal agency representatives provided updates on their respective agency programs, opportunities, and other activities. Meeting attendees had an opportunity to network and sign up for "speed coaching" with program officers from multiple agencies that discussed proposal preparation, funding opportunities, and other topics related to federal science and education programs.

International Collaboration in Chemistry (ICC) Program Update

Zeev Rosenzweig

The National Science Foundation (NSF) seeks to enhance opportunities for collaborative activities between U.S. and foreign investigators. To realize this goal, since 2006 the Division of Chemistry at NSF has partnered with a number of international funding agencies to enable the submission of collaborative proposals between US chemists and their counterparts abroad. This year, the ICC program welcomed the Binational Science Foundation (BSF) of Israel as a new ICC partnering agency. Details about the program, including a full list of participating partnering agencies, can be found in solicitation NSF 12-562: http://www.nsf.gov/pubs/2012/nsf12562/nsf12562.pdf

The ICC program funds research in all areas of chemistry that are supported by the Division of Chemistry. The proposals are submitted directly to individual investigator programs in the Division where they are reviewed and compared to thematically similar non-solicited proposals. Prospective PIs are encouraged to contact program directors in the individual investigator program aligned with their interests to discuss the suitability of their proposed project to that program prior to preliminary proposals submission. The ICC program gives higher priority to proposed projects that make use of resources and expertise that are only available in the foreign collaborator's laboratory. The program also encourages the submission of proposals in the area of sustainable chemistry.

Over the last two years, the Division has begun a process of graduating partnering agencies out of the ICC program to make room for new international partners. Last year, the Deutsche Forschungsgemeinschaft (DFG) of Germany was not listed as a partnering agency. This year, the Engineering and Physical Sciences Research Council (EPSRC) of the United Kingdom (UK) will not be listed as an ICC partner. US investigators who seek to collaborate with their counterparts in Germany or the UK may still do so by submitting an unsolicited proposal during our regular submission window for unsolicited proposals. More information about this change can be found in the revision page of the ICC solicitation NSF 12-562 (see link above).

The Division anticipates continuing the ICC program and even expanding opportunities to other countries in the coming years.

A Separation Science Symposium at ACS

Lin He

The NSF Division of Chemistry (CHE) and Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET), along with American Chemical Society (ACS) and the American Institute of Chemical Engineers (AIChE), co-sponsored a 1-day ACS symposium, titled "Ensuring the Sustainability of Critical Materials and Alternatives: Addressing the Fundamental Challenges in Separation Science and Engineering (SSE)."

The objectives of the symposium was to: 1) discuss the issues related to stresses in the global market and the key and enabling role of SSE in ensuring a sustainable supply and utilization of critical materials; 2) bring into focus crosscutting research needs and Scientific Grand Challenges in SSE associated with the sustainable extraction, recovery, recycling, and purification of critical materials; and 3) communicate these research needs to the SSE and broader science/engineering community.

The symposium was held Tuesday, August 21, at the 2012 Fall Meeting of the ACS in Philadelphia. It was co-chaired by Dr. Catherine T. Hunt (Dow Chemical Company) and Professor Mamadou S. Diallo (Caltech and KAIST). The symposium was designated an ACS Presidential event, hosted by the ACS Division of Analytical Chemistry, and co-sponsored by the ACS Committee on Environmental Improvement (CEI), the ACS Committee on Science (COMSCI), the ACS Committee on Corporation Associates (CA), and the ACS Division of Environmental Chemistry (ENVR). For additional information please see:

http://portal.acs.org/portal/acs/corg/content?_nfpb=true&_pageLabel=PP_MULTICOLUMN_T5_33&node_id=737&use_sec=false&sec_url_var=region1&__uuid=eb51c2a2-84aa-4201-967c-35c4fc5a4208

Division of Chemistry
Proposal Submission Window

Beginning in 2012, Chemistry Individual Investigator Award programs moved to a single window for each fiscal year. Depending upon the program, the window is either in September or in October.

Principal Investigators (PIs) may submit to the following programs between September 1st and September 30th in 2013:

- Chemical Catalysis - CAT
- Chemical Structure, Dynamics and Mechanisms - CSDM
- Chemical Theory, Models and Computational Methods - CTMC
- Chemical Synthesis - SYN

Proposals may be submitted to the following programs between October 1st and October 31st 2013:

- Chemical Measurement and Imaging - CMI
- Chemistry of Life Processes - CLP
- Environmental Chemical Sciences - ECS
- Macromolecular, Supramolecular and Nanochemistry - MSN

Note that if the last day of a submission window falls on a weekend or official federal government holiday, the deadline is always the following business day at 5 p.m. local time.

The CRIF, CAREER, REU, MRI, and the Centers for Chemical Innovation (CCI) programs and any other programs that have specified a submission date are not affected by this change. PIs should visit http://www.nsf.gov/div/index.jsp?div=CHE for the deadlines of these and other programs.

CHE discourages the submission of more than one proposal from the same PI during the proposal-submission window. Note that proposals that are a duplicate of, or substantially similar to, a proposal already under consideration by NSF from the same submitter are subject to return without review. This also applies to proposals that were previously reviewed and declined and have not been substantially revised, as well as duplicates of other proposals that have already been awarded.

Proposals directed to the Sustainable Chemistry, Engineering, and Materials (SusChEM) emphasis area should have a title that begins with "SusChEM:". For additional information on SusChEM, see http://www.nsf.gov/pubs/2012/nsf12097/nsf12097.jsp?org=NSF

Please contact program staff from the respective Division programs for additional information. http://www.nsf.gov/staff/staff_list.jsp?org=CHE&from_org=CHE.

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