WINTER 2017

DIVISION OF CHEMISTRY

CHE NEWSLETTER

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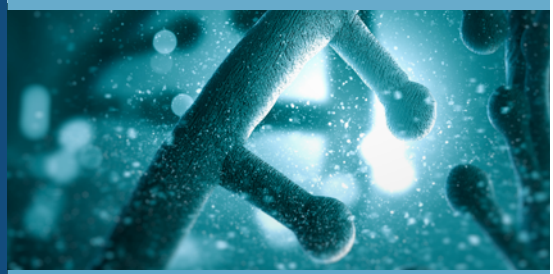

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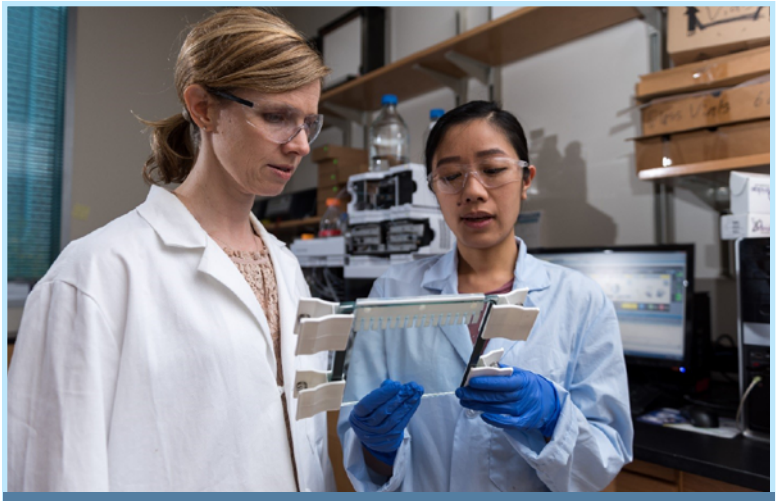

NSF GRFP student researcher Christine He shows Georgia Tech Associate Professor Martha Grover a gel used to separate nucleic acid strands. Both scientists are members of the Center for Chemical Evolution (CHE-1504217). Photo credit: Georgia Tech / Rob Felt.

VISCOSITY PROMOTES TEMPLATE-DIRECTED SYNTHESIS OF GENE-LENGTH RNA

With joint support from the Center for Chemical Innovation (CCI) Program in the Division of Chemistry (CHE) at NSF and the Astrobiology Program at NASA, the Center for Chemical Evolution (CCE) is researching the chemical origins of biopolymers. This research may represent a fundamental advance in the understanding of the chemical origins of life. In particular, CCE seeks to uncover how the earliest polymers of life spontaneously formed and initiated functional evolution billions of years ago.

In CCE, researchers in the laboratories of Professors Nicholas Hud and Martha Grover, both at Georgia Institute of Technology, collaborated on a project to determine how genetic information may have been transferred through replication of RNA in an enzyme-free, template-directed manner. This research was recently published in Nature Chemistry (doi:10.1038/nchem.2628). It addressed the issue of "strand inhibition"- a process where short denatured nucleotide chains reform into duplexes too quickly to allow for replication. While strand inhibition is a major problem in water, CCE researchers used a viscous solvent, glycholine, to slow down duplex reformation and demonstrate that solvent viscosity can enable information transfer from gene-length segments. These results suggest that viscous environments on prebiotic Earth, created by evaporation of aqueous pools containing small organic molecules, salts and oligonucleotides, could have enabled nucleic acid self-replication.

UPDATE FROM THE DIVISION DIRECTOR

After one year at NSF, I continue to be impressed with the administrative and technical staff at NSF. The Chemistry Division staff have a remarkable dedication to fund as much high quality, innovative science as possible.

The engagement of the chemistry community in the review process is also very much appreciated, and I thank all of you who have invested your time in the review process. Your involvement and insight are essential to achieving NSF's mission.

As you may know, NSF is moving from Arlington, Virginia to Alexandria, Virginia beginning in August 2017. The exterior of the new building has been completed and work has begun in earnest on the new panel and office spaces. Beginning October 1, 2017, our official address will be:

National Science Foundation
2415 Eisenhower Avenue
Alexandria, VA 22314

More information on the new space will be featured in our next quarterly Newsletter, however I wish to emphasize some of the implications that this move will have on the chemistry community, specifically regarding continuing grant increments.

Continuing Grant Increments (CGIs)

If you have an NSF grant for which you have received at least one year of funding, but not yet all of your funding, then you are asked to submit your annual report as soon as possible, but no later than June 2, 2017. For the move, NSF is closing out budgets earlier than in the past and we need to process CGIs efficiently. If you have any questions on this, please contact your Program Officer.

Workshops

The Division of Chemistry held a number of different workshops this past fall, targeting areas of interest to our community. Two workshops on possible needs for mid-scale instrumentation (i.e., instrumentation over $4 million (the current MRI limit) but under ~$70 M (the limit for Major Research Equipment and Facilities Construction), one on the quantum revolution (examining the utility of quantum phenomena, such as superposition and entanglement), and one on the chemistry of the brain. The workshop reports will be available on the CHE website by mid-summer.

A symposium that discussed highlights of the mid-scale instrumentation workshops was held on March 8, 2017 at the PittCon meeting in Chicago, IL.

Last year, the Division sponsored its first Chemistry Workshop for New Career Investigators to provide training on grant proposal preparation and the grant review process as well as interactions with successful investigators, and NSF Program Officers and Program Managers from other federal funding agencies. This year, the workshop is being organized by Professors Kate Plass (Franklin & Marshall College) and Tom Miller (California Institute of Technology). We plan to hold this workshop annually, so, junior faculty who may have missed the opportunity to attend this year are encouraged to apply for next year's workshop. Over 100 faculty participate in each workshop.

In terms of personnel, the Division often has openings for rotators. Frankly, I have found my experience as a rotator to be very rewarding. It is indeed possible to maintain your research laboratory while serving at NSF, as any of the Division of Chemistry rotators will attest. If you have an interest in considering a rotator opportunity at NSF or have any questions about the opportunity, please contact us at *che-recruit@nsf.gov*.

Angela K. Wilson
Division Director, CHE

ANNOUNCEMENTS

THE DIVISION WELCOMES THE FOLLOWING TECHNICAL STAFF MEMBERS

Catalina Achim

Dr. Catalina Achim, Professor of Chemistry at Carnie Mellon University has re-joined us as a part-time, off-site, Program Officer. She is assisting the Macromolecular, Supramolecular, & Nanochemistry (MSN) Program. Her research interests include hybrid inorganic-nucleic acid structures for nanotechnology and biological applications as well as polynuclear complexes with spin transitions for information storage applications.

John Papanikolas

Dr. John Papanikolas, Professor of Chemistry at the University of North Carolina, Chapel Hill has started his rotation as a Program Officer in the Macromolecular, Supramolecular and Nanochemistry (MSN) MSN and Chemical Structure, Dynamics, and Mechanisms (CSDM-A) Programs. Research in his group is directed at the characterization of complex chemical systems using femtosecond laser spectroscopy.

Gerald (GB) Hammond

Dr. Gerald (GB) Hammond, Endowed Chair in Organic Chemistry at the University of Louisville, has re-joined us as a part-time, off-site Program Officer in the Chemical Catalysis (CAT) Program. His research interests include new synthetic methodologies, organofluorine chemistry, gold catalysis, green chemistry and Peruvian medicinal plants.

Tong Ren

Dr. Tong Ren, Professor of Inorganic Chemistry, had re-joined us from Purdue University as a part-time, off-site Program Officer in the Centers for Chemical Innovation (CCI) and Chemical Structure, Dynamics, and Mechanisms (CSDM-A) Programs. Tong and his group are pursuing several research fronts rooted in synthetic and physical inorganic chemistry, with emphasis on compounds of importance in electronic and opto-electronic materials, biomimetic chemistry, and energy science.

HIGHLIGHTS

REQUEST FOR INFORMATION ON FUTURE NEEDS FOR ADVANCED CYBERINFRASTRUCTURE TO SUPPORT SCIENCE AND ENGINEERING RESEARCH

HTTPS://WWW.NSF.GOV/PUBS/2017/NSF17031/NSF17031.JSP?ORG=ICER

In the past two decades, advanced cyberinfrastructure has become a critical element of science and engineering research — a result of the increasing scope and accuracy of simulations of natural and engineered systems as well as the growing volume of data generated by instruments, simulations, experiments and observations. The National Science Foundation (NSF) embraces an expansive, ecosystem view of research cyberinfrastructure — spanning advanced computing resources, data and software infrastructure, workflow systems and approaches, networking, cybersecurity and associated workforce development — elements whose design and deployment are motivated by evolving research priorities as well as the dynamics of the scientific process. The critical role of this broad spectrum of shared cyberinfrastructure resources, capabilities and services — and their integration — in enabling science and engineering research has been reaffirmed by the National Strategic Computing Initiative, which was announced in July 2015, and in the National Academies' 2016 report on Future Directions for NSF Advanced Computing Infrastructure to Support U.S. Science and Engineering in 2017-2020. While these efforts are computing-centric, they expose the inherent inseparability of computing from the larger cyber ecosystem. NSF seeks input that provides a holistic view of the future needs for advanced cyberinfrastructure for advancing the Nation's research enterprise.

In 2009, NSF undertook a community-informed analysis of cyberinfrastructure needs that led to the formulation of a vision, a strategy, and a set of programmatic initiatives together comprising the current NSF-wide effort entitled ***Cyberinfrastructure for 21st Century Science and Engineering*** **(CIF21)** (see *https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504730*). Since that analysis, many changes have taken place in terms of scientific challenges and opportunities as well as technological progress. To continue to take full advantage of the potential provided by cyberinfrastructure to advance science and engineering research, NSF is beginning to formulate an updated strategy as well as concrete plans for future investments in this area. In this endeavor, NSF will focus on complementing and supporting forward-looking cyberinfrastructure for research that institutions and universities are unlikely to be able to deploy on their own. In addition, NSF seeks to stimulate innovative use of cyberinfrastructure for research to spur advances not otherwise possible, particularly in emerging areas of science and engineering research. Finally, NSF supports the exploration of approaches to sustainability that address the unique needs of research cyberinfrastructure, including the scientific, technical and human aspects of cyberinfrastructure.

Contributions must be made using the submission website *http://www.nsfci2030.org* on or before 5:00 PM Eastern time on April 5, 2017.

UPDATES TO FASTLANE:

PROPOSAL & AWARD POLICIES & PROCEDURES GUIDE (PAPPG) POLICY CHANGES AND NEW AND ENHANCED AUTOMATED COMPLIANCE CHECKS

HTTPS://WWW.NSF.GOV/PUBLICATIONS/PUB_SUMM.JSP?ODS_KEY=NSF17001

Effective January 30, 2017, NSF implemented the following changes in FastLane to support the policy updates in the ***Proposal & Award Policies & Procedures Guide*** (PAPPG) (NSF 17-1) and to run new and enhanced automated compliance checks on proposals:

PROPOSAL SUBMISSION

Two new types of proposals were incorporated into the PAPPG with new required supporting documents and automated proposal compliance checks:

> **Grant Opportunities for Academic Liaison with Industry (GOALI)**
>
> The new GOALI automated compliance checks require that at least one Co-Principal Investigator (PI) exists on the proposal and the "GOALI-Industrial PI Confirmation Letter" is uploaded at the time of proposal submission. All other automated compliance checks applicable to Research proposals also apply to GOALI proposals.
>
> **Research Advanced by Interdisciplinary Science and Engineering (RAISE)**
>
> The new RAISE automated compliance checks require that a "RAISE-Program Officer Concurrence Email" is uploaded at the time of proposal submission, the proposal award budget is less than or equal to $1 million, and the proposal duration is less than or equal to 5 years. All other automated compliance checks applicable to Research proposals also apply to RAISE proposals.

Proposers will be able to select GOALI and RAISE from the FastLane dropdown menu.

The Facilitation Awards for Scientists and Engineers with Disabilities (FASED) type of proposal also has been added to the FastLane dropdown menu. All automated compliance checks applicable to Research proposals will apply to FASED proposals.

Deadline Submission

The PAPPG includes additional instruction on how to submit proposals under the Special Exception to NSF's Deadline Date Policy. This section includes proposal preparation instructions for organizations impacted by a natural or anthropogenic disaster. Impacted proposers must check the "Special Exception to the Deadline Date Policy" box on the NSF Cover Sheet and upload the requisite Single Copy Document(s).

Updated References and Terminology

The PAPPG (NSF 17-1) has been modified in its entirety, to remove all references to the Grant Proposal Guide (GPG) and Award & Administration Guide (AAG). The document is now referred to solely as the NSF Proposal & Award Policies & Procedures Guide and is sequentially numbered from Chapter I-XII. All system references and links to the GPG and AAG have been updated to corresponding references and links in the PAPPG (NSF 17-1).

"International Travel" type of proposals was renamed to "Travel" and has been expanded to include domestic and international travel.

"Facility/Center" type of proposals was renamed to "Center/Research Infrastructure."

Enhanced Automated Compliance Checks

In addition to the new compliance checks for the GOALI, RAISE, and FASED types of proposals, FastLane will run enhanced automated compliance checks across several proposal types and will generate errors or warnings when the submission or deadline validation compliance checks are not met.

Checks are run during "Check Proposal," "Forward to SPO," and "Submit Proposal." The complete list of FastLane automated compliance checks effective January 30, 2017, are available online (see *https://www.nsf.gov/bfa/dias/policy/autocheck/compliancechecks_jan17.pdf*).

Note about Proposal File Update (PFU)

The automated compliance checks also apply when a PFU is performed on a proposal. The compliance checks will be run on all sections of the proposal, regardless of which section was updated during the PFU. Proposers should be aware that if a proposal was previously submitted successfully, a PFU performed on the proposal will be prevented from submission if the proposal does not comply with the compliance checks in effect at the time.

Note about Grants.gov

Grants.gov-submitted proposals are not compliance-checked by the FastLane system and therefore do not undergo the same set of automated compliance checks at submission as those submitted directly via FastLane. If NSF receives a proposal via Grants.gov that is not compliant, it will be returned without review.

CONTEXT STATEMENTS AND PROGRAM OFFICER (PO) COMMENTS

Often overlooked sources of information for Investigators — once your proposal has been recommended for award or declination — are the Context Statement and PO (Program Officer) Comments.

CONTEXT STATEMENT

Overall, the Context Statement may provide feedback about the number of awards that may be made in a given year. The Context Statement summarizes how many proposals came into the Division of Chemistry, separated out into categories such as Faculty Early Career Development (CAREER) and Research Experiences for Undergraduates (REU) Site proposals. The Context Statement includes the number of awards made and the funding rate for the previous year as well.

PO (PROGRAM OFFICER) COMMENTS

PO Comments are an official part of the review process and are used by your Program Officer to provide greater clarity regarding the award or decline decision of your proposal. PO Comments provide constructive feedback and, when appropriate, invite resubmission (after revision) or redirect resubmission. Program Officers use these comments to emphasize specific points that can be used by the PIs to improve their proposed research approach and/or presentation. These comments are provided for both declined and awarded proposals. CHE strongly recommends that all investigators read and consider these comments. They are located in Fastlane on the same page as your Reviews and Panel Summary (if applicable).

Office of the Division Director

Angela Wilson
Division Director

Carol Bessel
Deputy Division Director

Gloria Yancey
Program Support Manager

Debbie Jones
Operations Specialist

NO PHOTO

Michelle Jenkins
Program Analyst

Program Specialists Team

Marsha Hawkins
PS (CMI, MRI)

Irma Johnson
PS (CSDM-A & B, ECS)

Kimberly Noble
PS (CTMC, MSN)

Eric Pfeiffer
PA (CAT, CLP)

Marla Stewart
PS (Centers, SYN)

Technical Staff

Catalina Achim
PD (SYN)

Stephanie Albin
(AAAS Fellow)

Susan Atlas
PD (CTMC, Centers)

Michelle Bushey
PD (CMI, REU, Spec. Prj.)

Bob Cave
PD (CTMC, MRI, Centers)

Kelsey Cook
PD (CMI)

Katherine Covert
PD (Centers)

Colby Foss
PD (CSDM-A)

Max Funk
PD (CLP)

John Gilje
PD (SYN, CAT)

Evelyn Goldfield
PD (CTMC)

Gerald Hammond
PD (SYN)

Lin He
PD (CMI, Centers)

George Janini
PD (MSN)

Richard Johnson
Expert (SYN)

Bob Kuczkowski
PD (MRI)

Marjorie Langell
PD (MSN, CAT)

Tingyu Li
PD (CSDM-B)

Jim Lisy
PD (ECS, CTMC)

Kevin Moeller
PD (SYN, CAT)

Kenneth Moloy
PD (SYN, CAT)

Carlos Murillo
PD (MRI)

John Papanikolas
PD (MSN, CSDM-A)

Timothy Patten
PD (CAT, MSN)

Tong Ren
PD (Centers, CAT)

David Rockcliffe
PD (CLP)

Scott Rychnovsky
PD (CAT, SYN)

Anne-Marie Schmoltner
PD (ECS, CSDM-A)

Suk-Wah Tam Chang
PD (MSN)

CHE ORGANIZATION CHART

Division of Chemistry			
Name	**Title**	**Telephone**	**Email**
Dr. Angela Wilson	Division Director	703-292-4948	akwilson@nsf.gov
Dr. Carol Bessel	Deputy Division Director	703-292-4906	cbessel@nsf.gov
Mrs. Gloria Yancey	Program Support Manager	703-292-4718	gyancey@nsf.gov
Ms. Debbie Jones	Operations Specialist	703-292-7852	djones@nsf.gov
Ms. C. Michelle Jenkins	Program Analyst	703-292-7874	cjenkins@nsf.gov
Dr. Stephanie Albin	AAAS Fellow	703-292-2698	salbin@nsf.gov
Program Specialists Team			
Mrs. Marsha Hawkins	CMI, MRI	703-292-4877	mhawkins@nsf.gov
Ms. Illinois Johnson	CSDM-A&B, ECS	703-292-7182	ijohnson@nsf.gov
Ms. Kimberly Noble	CTMC, MSN	703-292-2969	knoble@nsf.gov
Mr. Eric Pfeiffer	CCI, DMREF	703-292-2977	epfeiffer@nsf.gov
Ms. Marla Stewart	CLP, SYN	703-292-8735	mastewart@nsf.gov
Technical Staff			
Dr. Catalina Achim	MSN	703-292-8840	cachim@nsf.gov
Dr. Susan Atlas	CTMC, CCI	703-292-4336	satlas@nsf.gov
Dr. Michelle Bushey	CMI, REU, Special Projects	703-292-4938	mbushey@nsf.gov
Dr. Robert Cave	CTMC, MRI, CCI	703-292-2394	rjcave@nsf.gov
Dr. Kelsey Cook	CMI	703-292-7490	kcook@nsf.gov
Dr. Katharine Covert	CCI	703-292-4950	kcovert@nsf.gov
Dr. Colby Foss	CSDM-A	703-292-5327	cfoss@nsf.gov
Dr. Max Funk	CLP	703-292-7441	mfunk@nsf.gov
Dr. John Gilje	SYN	703-292-8840	jwgilje@nsf.gov
Dr. Evelyn Goldfield	CTMC	703-292-2173	egoldfie@nsf.gov
Dr. Gerald Hammond	CAT	703-292-8840	ghammond@nsf.gov
Dr. Lin He	CMI, CCI	703-292-4956	lhe@nsf.gov
Dr. George Janini	CAT	703-292-4971	gjanini@nsf.gov
Dr. Bob Kuczkowski	MRI	703-292-8840	rkuczkow@nsf.gov
Dr. Marjorie Langell	MSN, CAT	703-292-8404	mlangell@nsf.gov
Dr. Tingyu Li	CSDM-B	703-292-4949	tli@nsf.gov
Dr. Kevin Moeller	SYN, CSDM-B	703-292-7054	kmoeller@nsf.gov
Dr. James Lisy	CTMC	703-292-2251	jlisy@nsf.gov
Dr. Kenneth Moloy	SYN, CAT	703-292-8441	kmoloy@nsf.gov
Dr. Carlos Murillo	MRI	703-292-4970	cmurillo@nsf.gov
Dr. Timothy Patten	CAT	703-292-7196	tpatten@nsf.gov
Dr. Tong Ren	CCI, CSDM-A	703-292-8840	tren@nsf.gov
Dr. David Rockcliffe	CLP	703-292-7123	drockcli@nsf.gov
Dr. Scott Rychnovsky	SYN, CAT	703-292-2170	srychnov@nsf.gov
Dr. Anne-Marie Schmoltner	ECS, CSDM-A	703-292-4716	aschmolt@nsf.gov
Dr. Suk-Wah Tam-Chang	MSN	703-292-8684	stamchan@nsf.gov

Chemistry Program Abbreviations	
Environmental Chemical Sciences (ECS)	Chemistry of Life Processes (CLP)
CHE Centers (CCI)	Designing Materials to Revolutionize & Engineer our Future (DMREF)
Chemical Catalysis (CAT)	Macromolecular, Supramolecular & Nanochemistry (MSN)
Chemical Measurement & Imaging (CMI)	Undergraduate Programs in Chemistry (REU)
Chemical Structure, Dynamics & Mechanisms (CSDM-A/B)	Chemical Theory, Models & Computational Methods (CTMC)
Chemical Synthesis (SYN)	Centers for Chemical Innovation (CCI)

DIVISION OF CHEMISTRY
National Science Foundation
4201 Wilson Boulevard, Arlington, Virginia 22230

For inquiries, comments or questions, please contact:
Marsha Hawkins Program Specialist, NSF/Chemistry
Phone: 703-292-4877 Email: mhawkins@nsf.gov