



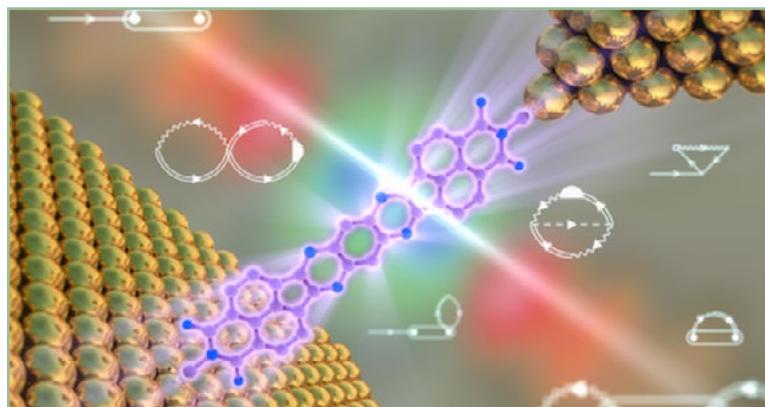
# CHE NEWSLETTER

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Galperin, Award **CHE-1565939**

## DEVELOPING A UNIFYING FRAMEWORK FOR MOLECULAR OPTOELECTRONICS

Optical spectroscopy has long been a first line molecular characterization method. As our technology has advanced to the nanoscale, experimentalists can now couple optical spectroscopy with single-molecule, current-carrying nanojunctions. This field, coined molecular optoelectronics, looks at the interaction of light and quantum electronic transport and transfer. While the field moves forward, with consideration of factors like transient measurements (pump-probe), hybrid light-matter states (polaritons), or quantum radiation (entanglement, squeezing, or photon counting), a unifying theoretical approach is necessary. Michael Galperin, at the University of California-San Diego, studies theoretical approaches at the intersection of quantum transport and optics. In a recent publication in *Chemical Society Reviews* (doi:10.1039/c7cs00067g) Galperin argues that the theoretical approach traditionally used in non-linear optical spectroscopy, bare perturbation theory formulated in Liouville space, falls short when nanojunctions are subject to bias or a quantized radiation field. Rather, he proposes that a non-equilibrium Green's function approach is a convenient tool to study quantum transport tied to either classical or quantum radiation. Adoption of a unifying theoretical framework may help the community gain greater insight into fundamental processes, and ultimately may help guide the design and development of molecular logic devices, sensors, or photovoltaics.

## CHE COMMUNICATION LISTSERV SIGN-UP

Stay informed with the latest news and topics of interest from the NSF Division of Chemistry: sign up for our mailing list by sending an email message with the subject line, 'Subscribe to CHE', to: [cheminfo@nsf.gov](mailto:cheminfo@nsf.gov). Please share this information with your colleagues!





## UPDATE FROM THE DIVISION DIRECTOR

Dear Colleagues,

It has been a busy and stimulating winter at NSF, with a lot of hallway “buzz” and conversations. Most of the conversations are about NSF’s 10 Big Ideas and the new research opportunities that have been developed. Some of these new opportunities are discussed later in this newsletter. I hope you find them as exciting as we do.

These *10 Big Ideas* are intellectual frontiers defined by our NSF Director, France Córdoba, and the National Science Board. Some of these *10 Big Ideas* sound less familiar to a chemistry audience, but I can assure you that there are opportunities for chemists in *Understanding the Rules of Life*, *The Quantum Leap*, *Harnessing the Data Revolution*, *Convergence Research*, *INCLUDES*, and *Mid-Scale Research Infrastructure*. Please take some time to read about a few of these and start conversations with your colleagues. Some of those conversations may turn into great proposals!

Meanwhile, the CHE staff is working through the more than 2000 research proposals submitted for consideration this fiscal year. More than 1700 of those proposals are submitted to the disciplinary research programs: individual-investigator proposals, small team proposals, GOALIs and RUIs. More than 80% of our funds will be spent on these “core” programs.

We think we do an excellent job reviewing these proposals and making funding recommendations in a challenging budget environment. But we always strive to do better! This year, we have been trying to improve the *PO Comments* by providing more specific guidance to PIs, particularly PIs that have been declined. You can find the PO Comments at the top of the FastLane Proposal Status page (where you find the reviews). Please let me know if you find them useful.

Interacting with the CHE PI community is a pleasure. I particularly enjoyed the 2018 Chemistry Early Career Investigator Workshop, held in late March in Alexandria, VA. Some of the newest members of our PI community took the opportunity to talk with CHE Program Directors, get advice on their proposal idea, and glimpse the way that proposals are evaluated at NSF. There was also time for networking with the NSF staff, more established chemistry faculty, and the many new faculty participants. Special thanks to workshop organizers Matt Whited (Carleton College) and Gordana Dukovic (Colorado), and CHE Program Director Anne-Marie Schmoltnner.

**Angela K. Wilson**  
Division Director, CHE

## CHEMISTRY STAFF NEWS AND RECRUITING

### WELCOME!



#### Catalina Achim

Dr. Catalina Achim is a Professor of Chemistry at Carnegie Mellon University. Her research areas are supramolecular chemistry, metal-containing peptide nucleic acids, electron transfer, molecular electronics, coordination complexes with

spin transitions, Mossbauer spectroscopy, molecular magnetism, and molecular-based materials. Dr. Achim has created the *DNAzone for K-12*. She has rejoined the division as a Program Director, and will be working in the Chemistry of Life Processes (CLP) and Macromolecular, Supramolecular & Nanochemistry (MSN) Programs.



#### Renee Ivey

Ms. Renee Ivey is working in the Division on a 120 day detail assignment as a Program Specialist working with the Chemical Catalysis (CAT) and Chemistry of Life Processes (CLP) programs.

### CONGRATULATIONS!



#### Kenneth Moloy

Dr. Kenneth Moloy, formerly a Research Fellow in the Central Research and Development department at E.I. DuPont de Nemours & Company, is now a permanent Program Director. He currently works in the Chemical Catalysis (CAT) and Chemical

Synthesis (SYN) Programs.



#### Timothy Patten

Dr. Timothy Patten, formerly a Program Director in Chemistry, is now the Deputy Division Director for the Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET) within the Engineering Directorate (ENG).

An updated *staff list* is available on the CHE webpage.

### CONSIDERING JOINING THE NSF STAFF?

An integral subset of our program directors are rotators, members of the chemistry community that serve at NSF for 1-4 years. Rotators bring in fresh perspectives from their research community, oversee NSF's merit review process, make award recommendations, and help to guide the division's portfolio balance and initiatives. They also have a unique opportunity to survey their field and gain a more multi-disciplinary lens, build leadership skills, and mentor the next generation of investigators. While serving as a program director at NSF, rotators may also continue their research at their home institution through the Independent Research/Development program.

The Division of Chemistry is actively recruiting program directors with experience in all fields of chemistry, especially those with an expertise in physical chemistry or inorganic synthesis. Please reach out to our current staff with any questions, visit the *Career Opportunities* section on our division website for information on how to apply, or visit the *NSF Careers home* for more information on being a rotator.

## BIG IDEAS & FUNDING OPPORTUNITIES

NSF's *10 Big Ideas* ([https://www.nsf.gov/news/special\\_reports/big\\_ideas/index.jsp](https://www.nsf.gov/news/special_reports/big_ideas/index.jsp)) identify bold, long-term research and process ideas that identify areas for future investment at the frontiers of science and engineering. The *10 Big Ideas* represent unique opportunities to position our Nation at the cutting edge of global science and engineering leadership and to invest in fundamental research and processes that advance U.S. prosperity, security, health, and well-being.

The chemistry community is strongly encouraged to participate in all of the *10 Big Ideas*. The following is a sampling of specific opportunities with upcoming deadlines for FY 2018.

### HARNESSING THE DATA REVOLUTION

With recent advances in technology and computing infrastructure, many fields of science and engineering now have access to vast amounts of data, enabling data-driven innovation and leading to new data-driven research challenges. The challenges posed by complex data elements such as images, text, and networks; unstructured and heterogeneous data formats; streaming and dynamic data; complex dependence structures; missing, uncertain, and noisy information; sparsity; and information hidden at the noise level will require research that

- a) addresses the core algorithmic, mathematical and statistical principles and
- b) leads to new approaches, computational tools, and software for data-driven discovery within and across science and engineering domains.

More ideas and context are available in the new workshop report: Framing the Role of Big Data and Modern Data Science in Chemistry: [https://www.nsf.gov/mps/che/workshops/data\\_chemistry\\_workshop\\_report\\_03262018.pdf](https://www.nsf.gov/mps/che/workshops/data_chemistry_workshop_report_03262018.pdf). Our thanks to the workshop organizers: Johannes Hachmann, Theresa Windus, and John McLean, as well as all of the workshop participants.

### TRIPODS + X (NSF 18-542)

[HTTPS://WWW.NSF.GOV/PUBLICATIONS/PUB\\_SUMM.JSP?ODS\\_KEY=NSF18542](https://www.nsf.gov/publications/pub_summ.jsp?ods_key=NSF18542)

In FY 2017, the Directorates for Computer and Information Science and Engineering (CISE) and Mathematical and Physical Sciences (MPS) launched the Transdisciplinary Research in Principles of Data Science (TRIPODS) Phase I with 12 awards [https://www.nsf.gov/news/news\\_summ.jsp?cntn\\_id=242888](https://www.nsf.gov/news/news_summ.jsp?cntn_id=242888).

The recently released TRIPODS + X solicitation seeks to expand the scope of the TRIPODS program by engaging researchers in chemistry and other domain disciplines across NSF. Working in concert with an existing TRIPODS organization, a TRIPODS + X project would focus on data-driven research challenges motivated in one or more science and engineering domains aimed at building robust data science communities.

Example topics include: understanding the correlations between synthesis and physical properties through data science or data-driven discoveries to advance fundamental understanding of chemical systems.

At least one PI or Co-PI or Senior Personnel must represent one of the 12 TRIPODS Phase I Institute projects (see above) and at least one PI or Co-PI must represent a domain discipline (such as chemistry).

Deadline May 29, 2018. Questions about TRIPODS + X may be directed to Lin He, Division of Chemistry, 703-292-4956 or [lhe@nsf.gov](mailto:lhe@nsf.gov).

**DATA-DRIVEN DISCOVERY SCIENCE IN CHEMISTRY (D3SC, NSF 17-112)**

[HTTPS://WWW.NSF.GOV/PUBS/2017/NSF17112/NSF17112.PDF](https://www.nsf.gov/pubs/2017/nsf17112/nsf17112.pdf)

CHE encourages the submission of D3SC EAGER, RAISE and supplemental funding requests. The D3SC DCL supports data-driven discoveries to advance fundamental understanding of chemical systems.

Here is a list of last year's D3SC EAGER awards with links to the award abstracts:

Grant #	Grant Title	PI
1738975	D3SC: EAGER: Collaborative Research: A probabilistic framework for automated force field parameterization from experimental datasets	Michael Shirts
1738979	D3SC: EAGER: Collaborative Research: A probabilistic framework for automated force field parameterization from experimental datasets	John Chodera
1738305	D3SC: EAGER: Data-driven development of fluorescent sensors for bio-imaging	Ming Xian
1734082	D3SC: EAGER: Using Deep Learning to Find Algorithms for Optimizing Chemical Reactions	Richard Zare
1738990	D3SC: EAGER: Data-driven design of molecular models from microscopic dynamics and experimental data	Cecilia Clementi
1709351	CDS&E: D3SC: The Dark Reaction Project: A machine-learning approach to exploring structural diversity in solid state synthesis	Joshua Schrier

**THE QUANTUM LEAP**

*The Quantum Leap* aims to exploit quantum mechanical phenomena such as superposition and entanglement to develop next-generation technologies for sensing, computing, modeling, and communication.

In the Fall of 2016, the Division of Chemistry sponsored a workshop entitled "*Quantum Information and Computation for Chemistry*", led by Alán Aspuru-Guzik of Harvard University and Michael Wasielewski of Northwestern University to explore the relevance of Quantum Leap to the field of chemistry. The workshop identified areas where chemists can contribute to advancing *The Quantum Leap* and areas where advances in *The Quantum Leap* can enable the solution of intractable chemical problems.

**ENABLING QUANTUM LEAP IN CHEMISTRY (QLC, NSF 18-051)**

[HTTPS://WWW.NSF.GOV/PUBS/2018/NSF18051/NSF18051.PDF](https://www.nsf.gov/pubs/2018/nsf18051/nsf18051.pdf)

To follow up on the recommendations of the workshop, CHE invites supplemental funding requests and EAGER proposals that explore molecular approaches towards problems in quantum computing, sensing, communicating, etc. A partial list of topics is given in the Dear Colleague Letter (DCL), and additional topics are explored in the workshop report.

If you are interested, we strongly encourage you to contact the cognizant program officers prior to submission to determine the appropriateness of the work for consideration by sending email to [QLChem@nsf.gov](mailto:QLChem@nsf.gov). The supplemental funding requests and EAGER proposals must be submitted by **May 1, 2018, 5:00 pm, submitter's local time**.

## UNDERSTANDING THE RULES OF LIFE

*Understanding the Rules of Life* will explore how we predict the phenotype, the structure, function and behavior of an organism, based on what we know about its genes and environment. With improved understanding, we may be able to predict how cells, brains, bodies and biomes will respond to changing environments.

### DESIGN AND ENGINEERING OF SYNTHETIC CELLS AND CELL COMPONENTS (DESYN-C<sup>3</sup>, NSF 18-071)

[HTTPS://NSF.GOV/PUBS/2018/NSF18071/NSF18071.JSP](https://NSF.GOV/PUBS/2018/NSF18071/NSF18071.JSP)

This DCL describes an initial opportunity to expand and test our current understanding through the design of synthetic cell components (ribosomes, mitochondria, membranes, regulators, molecular machines, etc.) and molecular probes, and their synthesis and integration into “pseudo-cells” that efficiently convert raw materials to useful products.

NSF is welcoming proposals to support Conference, EAGER and RAISE projects. See the *NSF Proposal & Award Policies & Procedures Guide (PAPPG)* for more information about these three types of proposals (**NSF PAPPG 18-1, Chapter II. E**). For more information please contact Catalina Achim ([cachim@nsf.gov](mailto:cachim@nsf.gov)) or Susan Atlas ([catlas@nsf.gov](mailto:catlas@nsf.gov)).

## CONVERGENCE RESEARCH

Convergence Research is a means of solving vexing research problems, in particular, complex problems focusing on societal needs. It entails integrating knowledge, methods, and expertise from different disciplines and forming novel frameworks to catalyze scientific discovery and innovation.

### GROWING CONVERGENCE RESEARCH (NSF 18-058)

[HTTPS://WWW.NSF.GOV/PUBS/2018/NSF18058/NSF18058.JSP](https://WWW.NSF.GOV/PUBS/2018/NSF18058/NSF18058.JSP)

Research relying on convergence is needed to solve complex scientific and engineering problems that require integrating knowledge, methods, and expertise from different disciplines and forming novel frameworks to catalyze scientific discovery and innovation. *Convergence Research* has two primary characteristics:

- **Research driven by a specific and compelling problem.** Research requiring a convergence paradigm is generally inspired by the need to address a specific challenge or opportunity, whether it arises from deep scientific questions or pressing societal needs.
- **Deep integration across disciplines.** As experts from different disciplines pursue common research challenges, their knowledge, theories, methods, data, research communities and languages become increasingly intermingled or integrated. New frameworks, paradigms or disciplines can form from sustained interactions across multiple communities.

The Growing Convergence Research DCL encourages submission of RAISE proposals (up to \$1.0 million for three years); deadlines are May 1, 2018 and Oct 15, 2018. The topics are open in this call, but topics related to one or more of the *10 Big Ideas* are especially encouraged.

## CHEMISTRY FUNDING OPPORTUNITIES

### CENTERS FOR CHEMICAL INNOVATION (CCI PHASE I, NSF 18-555)

[HTTPS://WWW.NSF.GOV/FUNDING/PGM\\_SUMM.JSP?PIMS\\_ID=13635&ORG=CHE&SEL\\_ORG=CHE&FROM=FUND](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=13635&org=che&sel_org=che&from=fund)

NSF Chemistry is offering the CCI Phase I opportunity again in FY 2019. Some key changes:

- Earlier deadline for preliminary proposals, in mid-August 2018.
- Particular encouragement for topics related to one or more of the NSF's *10 Big Ideas*.

CCI Phase I awards are the first step in building a major research center focused on a chemistry research challenge. If you are interested, please see NSF 18-555 and consider talking with one of the cognizant Program Directors.

### SUPPLEMENTAL FUNDING OPPORTUNITIES

PIs are encouraged to discuss supplemental funding requests with a cognizant Program Officer before submission. The *NSF PAPPG* Chapter VI.E.4, provides specific guidance on preparing a supplemental funding request.

#### IMPROVING GRADUATE STUDENT PREPAREDNESS (NSF 18-056)

[HTTPS://WWW.NSF.GOV/PUBS/2018/NSF18056/NSF18056.JSP](https://www.nsf.gov/pubs/2018/nsf18056/nsf18056.jsp)

The Division of Chemistry (CHE) supports masters and doctoral students to acquire the knowledge, experience, and skills needed for highly productive careers. This Dear Colleague Letter describes opportunities for supplemental funding (up to \$12K) to enhance the training experience of graduate students supported by active CHE research grants who are considering careers outside of academe. Please see the DCL for additional guidance. Supplemental funding requests should be submitted no later than **May 1, 2018**.

## FOR PROPOSERS: IMPROVEMENTS AND REMINDERS

- **FastLane and Research.gov IDs and Passwords**  
The next time you are in *FastLane or Research.gov*, you may be asked to update your *ID and password*. For more info, see the “About Account Management” page accessible on the Research.gov homepage.
- **Research.gov Proposal Preparation and Submission**  
Beginning on April 30, 2018, proposers will be able to prepare and submit full, research non-collaborative proposals in *Research.gov*. This is a very exciting first step to modernize *proposal preparation and submissions* in *Research.gov*. Key features include the use of real-time compliance checks, inline help tips and notes, and a proposal wizard that will walk users through the proposal set up process. Sneak peeks available now on the preview site, but remember that you can't save your data on the preview site.
- **Collaborators and Other Affiliations**  
NSF requires that all proposal submissions include a completed Collaborators and Other Affiliations (COA) template, which can be found at: <https://nsf.gov/bfa/dias/policy/coa.jsp>. Information about your PhD advisor(s), your current and former PhD thesis advisees, as well as all individuals whom you have collaborated with or coauthored a book, article, report, abstract or paper in the 48 months prior to proposal submission should be listed in the COA template, and NOT in the Biographical Sketch section of the proposal. Incomplete COA templates will cause delays in the review of your proposal, and possibly even a return of the proposal without review.
- Want to know what your Program Officer *really* thinks about your proposal? This is a time of year when many PIs are accessing proposal reviews via *FastLane's Proposal Status* page. That feedback can be critical for further developing a project. Did you know that your Program Officer is also providing feedback?
- There is a short section called “*Comments from the cognizant Program Officer*” at the top of the same page (above the review links). They are only a few sentences long, but try to capture key points in the program's recommendation. This isn't the only way you can find out what is on your Program Officer's mind; you can always set up a time to talk about your proposal's review and recommendation. We recommend that you send your PO an email (the email address will be on the Proposal Status page, as well), with some proposed dates and times for a full discussion.

## FOR FUNDED PIS: UPDATE ON PUBLIC ACCESS & REPORTING REQUIREMENTS

As part of a government-wide effort to provide more public access to the results of Federal funding, NSF established a *Public Access Repository* (NSF-PAR, <https://par.nsf.gov/>). For more information on NSF's public access requirement, see *the “About Public Access” page on Research.gov*.

This spring is the first time CHE awardees are being impacted by this new requirement. If you have a new award (or newly renewed award) from FY 2017, you will be required to use NSF-PAR.

## FOR OUR PANELISTS: TRAVEL UPDATES

- The NSF Website has updated information on our new Alexandria location <https://www.nsf.gov/about/visit/>
- New GSA mileage reimbursement: \$0.545 per mile. If you are planning to drive to an NSF panel, please contact the Program Specialist working with your panel.

## CHE ENGAGING THE RESEARCH COMMUNITY

- **256th American Chemical Society (ACS) National Meeting**

The 256th American Chemical Society (ACS) National meeting will be held in Boston, MA at the Boston Convention and Exhibition Center from August 19th-23rd, 2018. The Division of Chemistry plans to hold a meet-and-greet luncheon where Chemistry staff members will be available to discuss funding and research opportunities, broadening participation and education, and outreach. Attendance is free, with box lunches available for purchase. Please watch the Governance and Social Events portion of the ACS conference program and the CHE website for more details.

- **45th Annual Meeting, National Organization for the Professional Advancement of Black Chemists and Chemical Engineers (NOBCChE)**

Members of the Division of Chemistry will attend NOBCChE's 45th Annual Meeting, September 17-20, 2018, in Orlando, Florida. CHE staff will attend the Career Fair, and will provide information on NSF's funding opportunities that are available for students, such as the Research Experiences for Undergraduates (REU) Program; the Louis Stokes Alliances for Minority Participation (LSAMP) Program; and the Graduate Research Fellowship Program (GRFP).

CHE staff will also give presentations on various funding mechanisms in/outside of Chemistry; international collaborations; additional supplemental funding opportunities for students and Principal Investigators, as well as an overview on Chemistry's program structure and the lifecycle of a proposal submitted to Chemistry.

More details (as they are available) on Chemistry's [website](#) and the NOBCChE meeting agenda.

- **2018 NSF Chemistry Early-Career Investigator Workshop**

On March 26 and 27, 2018, one hundred early-career chemists met in Alexandria, VA, to learn about funding for chemistry research at NSF. The workshop was organized by Profs. Matthew Whited (Carleton College) and Gordana Dukovic (University of Colorado, Boulder). The participants learned about NSF from panels presented by program officers, round table discussions, and one-on-one meetings. Several CAREER awardees shared their experience and advice on proposal writing. The participants had the opportunity to participate in mock panels, and practice their skills in communicating science to a non-expert audience. Program Officers from other divisions at NSF as well as the DOE, NIH, AOR, and AFOSR engaged with participants who were interested in finding out more about other funding opportunities.



Workshop attendees and NSF staff at the 2018 ECI Workshop. Image credit: Anne-Marie Schmoltner

## CHE ON THE WEB

- We are regularly publishing research highlights on NSF's Tumblr page, a repository for brief research highlights across all NSF funded projects. You can find chemistry highlights by scrolling through the main *NSF Tumblr page* or by going directly *here*.

While a Tumblr account is not necessary to view content, it is required to 'like' or re-blog a post. Tumblr may also be added to an RSS feed to receive alerts on each new post. We also invite our investigators to submit their own highlights by following the directions *here*.

- Funding information, deadlines, and highlights for the Division of Chemistry are also regularly posted on the Directorate for Mathematical and Physical Sciences Twitter account. These posts, or tweets, can be found *here*, or under the Twitter handle @NSF\_MPS. A Twitter account is not necessary to view the content, but is needed to receive updates or to interact with a tweet.

## BROADER IMPACTS IN ACTION



A part of the Division of Chemistry's mission is realizing the broader impacts of our funded science, including community engagement in the real-world chemistry that surrounds us. Every year educators bring the scientific method to life and into communities through science fairs, where children get to choose a scientific topic for investigation. This past year in Florida, middle-schooler Charlie Schuessler wanted to investigate a serious local problem – sink hole formation. Sinkholes generally form as water slowly dissolves the bedrock, often made of limestone, so Charlie wanted to know if there was any sort of way to stop or slow limestone dissolution. Charlie and his mother turned to the internet for background research when they came across CHE-funded investigator Professor Jonas Baltrusaitis at Lehigh University. As a part of his postdoctoral work at the University of Iowa, Professor Baltrusaitis studied hydrophobic coatings to preserve historical, lime-stone clad buildings. He found that moisture coupled with air pollution, particularly sulfur oxides, lead to limestone degradation, but that degradation could be slowed with hydrophobic coatings. With Professor Baltrusaitis's help, Charlie designed an experiment to compare the dissolution of limestone with and without a commercial hydrophobic coating. Charlie found the hydrophobic coating did have a small effect in protecting the limestone, and even won his science fair. Charlie's mother, Cassie, said the judges "were impressed that he had involved an expert in his research."

*Information on the above photo: Charlie Schuessler and his science project. (Image credit to Carrie Schuessler, Charlie's mother)*

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Chemistry Program Abbreviations			
Chemical Catalysis (CAT)	Environmental Chemical Sciences (ECS)		
CHE Centers (CCI)	Major Research Instrumentation (MRI)		
Chemistry of Life Processes (CLP)	Macromolecular, Supramolecular & Nanochemistry (MSN)		
Chemical Measurement & Imaging (CMI)	Research Experiences for Undergraduates (REU)		
Chemical Structure, Dynamics & Mechanisms (CSDM A & B)	Chemical Synthesis (SYN)		
Chemical Theory, Models & Computational Methods (CTMC)			

The mission of the Division of Chemistry is to promote the health of academic chemistry and to enable basic research and education in the chemical sciences. The Division supports research in all traditional areas of chemistry and in multidisciplinary fields that draw upon the chemical sciences. The Division also supports projects that help build infrastructure, workforce, and partnerships that advance the chemical sciences.

**DIVISION OF CHEMISTRY**  
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