



# CHE NEWSLETTER

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## 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!



*PI: Michael J. Zdilla — Temple University, CAREER award CHE-1254545  
Graduate student researcher Michael Gau demonstrates the safe handling of tert-butyllithium reagents in the first open access, peer-reviewed video protocol for the safe use of pyrophoric (spontaneously igniting) lithium chemicals.*

## A PROTOCOL FOR SAFE LITHIATION REACTIONS USING ORGANOLITHIUM REAGENTS

Organolithium reagents are powerful bases and extremely useful in organic and inorganic syntheses. A major concern with the use of these important reagents is safety, since when improperly handled, they can result in fire, burns and death. In 2008, a student in a synthetic chemistry laboratory at the University of California died as a result of burns she received while using tert-butyllithium sparking worldwide concern and trepidation about the use of this reagent. Unfortunately, the tragedy could have been avoided if very simple protocols had been followed. As with any specialized technique, the best way to learn is to watch an expert.

Dr. Zdilla has provided a video protocol that visually illustrates the proper handling of these important reagents so that anyone with undergraduate-level synthetic chemistry training can perform reactions with the reagent safely. This open source protocol serves as a training resource for any researcher needing these powerful reagents, can be used to attenuate the unnecessary fear surrounding the use of these reagents, and can lessen the likelihood of the occurrence of future accidents, ultimately saving lives.

Watch the video for free here: <https://www.jove.com/video/54705/a-protocol-for-safe-lithiation-reactions-using-organolithium-reagents>



## UPDATE FROM THE DIVISION DIRECTOR

Dear Colleagues,

We hope that you have had an enjoyable summer! We have had a busy summer, finishing 2017 awards, and planning for 2018 and 2019, as well as preparing for our move. In August, NSF moves to its new home in Alexandria, Virginia, conveniently located next to the Eisenhower Metro Station. The facility is very nice, and includes a business center for visiting panelists. We look forward to welcoming you to the new facility.

There are several items to which we would like to draw your attention, many of which are highlighted later in this newsletter: Congratulations to the 2017 Division of Chemistry CAREER Awardees! The awardees represent a broad spectrum of research interests and universities, and we look forward to hearing about their research endeavors. For those who plan to submit CAREER proposals during Summer 2018 or later, the Division of Chemistry plans to support another Early Career Workshop during Spring 2018 for junior faculty. More details will become available later in the fall on the NSF Chemistry (CHE) website.

If you will be submitting proposals in 2017 or 2018, note that CHE has revised its data management plan guidance, and the updated guidance can be found online by clicking this link: <https://www.nsf.gov/bfa/dias/policy/dmpdocs/che.pdf>. In addition, all the CHE programs have newly revised program descriptions that provide more insight about topics funded for each of the programs.

Over the past year, CHE hosted a number of workshops, including workshops on data science and discovery in chemistry, Quantum Leap (new and emerging areas in quantum science), mid-scale instrumentation (chemistry instrumentation that would cost more than \$4M, but less than \$70M), and chemistry of the brain. These workshop reports are available via the CHE website.

Earlier this year, CHE had its first Dear Colleague Letter (DCL) on Data-Driven Discovery Science in Chemistry (D3SC). There was significant interest in the program from the community, and very exciting proposals were submitted from a broad range within the chemistry community, including proposals from both the experimental and theoretical components of our discipline. CHE is continuing this DCL grant opportunity, and welcomes proposals for this program.

This past year, CHE had a solicitation for Phase I Centers for Chemical Innovation (CCI). The CCI program supports investigators who collectively pursue a grand challenge in chemistry at the level of \$1.8M total over three years. Phase I Centers can subsequently compete for Phase II awards, which are up to \$4M/year for five years, and have the potential for renewal for up to five additional years. We encourage you to consider this opportunity.

CHE staff will be actively participating in the ACS Fall National Meeting in Washington DC. NSF will participate in the Federal Funders Town Hall Meeting on Monday afternoon, where I will discuss the current state of NSF, CHE funding and opportunities. Other agencies will also be speaking at the event. Earlier in the day, federal agencies and other funding organizations (i.e., private foundations and companies) that provide financial support for research will participate in a poster session about funding opportunities in their organizations.

Finally, when I started at NSF, I had agreed to stay approximately two years and then return to my home institution (and my research group!) at Michigan State University. We now are beginning our search for a new Division Director for the position opening in 2018. I have very much enjoyed my time at NSF and highly recommend the opportunity. (I can also assure you that it is possible to manage a research program from afar.) The leadership and learning experiences have been enjoyable, and the NSF CHE staff are a terrific group of people with whom to work. Please contact Angela K. Wilson if you would like to discuss the opportunity. We welcome nominations and self-nominations. We are also always looking for rotator program director, and if you wish to be involved in CHE in a rotation as a Program Director please contact us at 703-292-8840 or email: [che-recruit@nsf.gov](mailto:che-recruit@nsf.gov).

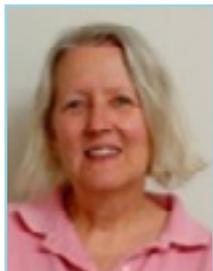
I hope that you have an enjoyable rest of the summer and a terrific fall!

Sincerely,

Angela K. Wilson  
Division Director, CHE

## CHEMISTRY STAFFING ANNOUNCEMENTS

THE DIVISION WOULD LIKE TO SAY GOODBYE TO THE FOLLOWING STAFF MEMBERS



The Division would like to say thank you to Dr. Marjorie Langell for her dedication and hard work as Program Director for the Macromolecular, Supramolecular and Nanochemistry (MSN) and Chemical Catalysis (CAT) Programs. The Division of Chemistry wishes her continued

success. Dr. Marjorie Langell will return to the University of Nebraska-Lincoln.



The Division would like to say thank you to Dr. Scott Rychnovsky for his dedication and hard work as Program Director for the Chemical Catalysis (CAT) and Chemical Synthesis (SYN) Programs. The Division of Chemistry wishes

him continued success. Dr. Scott Rychnovsky will return to the University of California-Irvine.

THE DIVISION WOULD LIKE TO CONGRATULATE THE FOLLOWING STAFF MEMBER



Illinois (Irma) Johnson will start a 120-day detail in the Office of Integrative Activities (OIA). Starting on June 25, 2017, Irma will work in the Evaluation Assessment and Capability Section (EAC) as a Program Analyst. Good luck Irma with your new opportunity!

## RELOCATION OF THE NATIONAL SCIENCE FOUNDATION (NSF)



The NSF Headquarters will prominently reflect NSF's role in the science and engineering community, nationally and internationally. The goal is to create a totally -user-friendly environment that integrates people (culture), tools (technology) and place (work environment) in a manner that reflects NSF's status as the premier science agency of the United States Government.

One great thing about the move is that the employees will be able to keep their same phone numbers!

The Division of Chemistry will be moving to the new headquarters in early September.

**New HQ Address:**

National Science Foundation  
2415 Eisenhower Avenue  
Alexandria, VA 22314

# REVISED DATA MANAGEMENT PLAN GUIDANCE

DIVISION OF CHEMISTRY UPDATED ADVICE TO PRINCIPAL INVESTIGATORS ON DATA MANAGEMENT PLANS | JUNE 26, 2017

The Division of Chemistry (CHE) offers the following guidance for CHE investigators to consider when developing required Data Management Plans (DMPs) for their proposal submissions. This document is a supplement to the data management plan requirements summarized in the Proposal & Award Policies & Procedures Guide (PAPPG)<sup>1</sup>, and has been developed to aid Principal Investigators (PIs) in Chemistry in developing effective, complete, and competitive DMPs. It is important to recognize that while all DMPs should address the five categories of information specified in the PAPPG, they should not be generic. Each DMP should be appropriate for the particular set of data, metadata, samples, software, curricula, documentation, publications, and other materials generated in the course of the proposed research. DMPs should reflect best practices and standards for the proposed research and types of data being generated, whether experimental, computational, or text-based. DMPs are subject to peer review. Please contact a CHE Program Officer if you have any questions related to DMPs in the program context.

For more information on the history of the DMP requirement, and NSF's expectations for the dissemination and sharing of research results, see this document's appendix.

## PAPPG AND NSF-WIDE REQUIREMENTS

All proposals must include a supplementary document of no more than two pages labeled "Data Management Plan," as described in the **PAPPG Part I Section II.C.2.j**. Any specific instructions and exceptions to the two-page limit will be found in specific Program Solicitations.

A proposal without a supplementary DMP will not be accepted<sup>2</sup>.

A valid DMP may include only the statement that no detailed plan is needed, provided that the statement is accompanied by a clear justification<sup>3</sup>.

If proposers feel that the DMP cannot fit within the 2-page limit, they may also use part of the 15-page Project Description for additional data management information<sup>4</sup>.

- Any costs associated with implementing the DMP should be explained in the Budget Justification<sup>5</sup>.
- The DMP will be reviewed as an integral part of the proposal, considered under Intellectual Merit or Broader Impacts or both, as appropriate for relevance to the scientific community.

## DMP CONTENT

CHE-supported research covers a broad spectrum of communities of investigators, and each community has its own best practices. CHE is aware of the need to provide flexibility to reviewers and Programs in assessing the quality of individual DMPs. The standards for DMPs are evolving to accommodate changing standards and expectations, and CHE relies on the merit review process to determine which DMPs best serve each community. CHE will continually revise this Advice document accordingly.

The DMP should clearly articulate how the investigators plan to manage and disseminate data generated by the project, taking advantage of emerging information technologies and cyberinfrastructure. **The plan must include sufficient detail for evaluation of its appropriateness and feasibility during merit review.** DMPs often include existing practices of the principal investigator's laboratory and the larger research community. CHE strongly encourages innovation that, where appropriate and practical, enables efficient and effective data sharing and management to stimulate and promote scientific advances.

1 This document refers to the PAPPG effective January 30 2017, document number [NSF 17-001](#). Please check to see if there are significant changes and clarifications to the PAPPG since the publication of this document.

2 [https://www.nsf.gov/bfa/dias/policy/autocheck/compliancechecks\\_jan17.pdf](https://www.nsf.gov/bfa/dias/policy/autocheck/compliancechecks_jan17.pdf)

3 In the case of a workshop or REU proposal, the DMP should discuss the management of data that may be generated as part of the proposed activity (e.g. participant lists, exit surveys, community reports).

4 A DMP that lacks detail and simply states "see project description" will likely not be considered sufficient.

5 "As long as the costs are allowable in accordance with the applicable cost principles, and necessary to implement the DMP, such costs may be included (typically on Line G2) of the proposal budget, and justified in the budget justification." From [Data Management & Sharing FAQs](#)

In what follows, the five essential components of the DMP are listed in the same order as in the PAPPG, with examples relevant for the Chemistry community. **Note: these examples are not intended to supplant the guidance given in the PAPPG.**

### 1. Products of the Research

This section describes the types of data (including metadata and annotations, primary or analyzed) and products that will be generated by the research, for example description of samples, numerical data on chemical systems such as spectra, chemical and physical properties, time-dependent information on chemical and physical processes, theoretical formalisms, experimental protocols, algorithm specifications, database schemas and data tables, data produced by simulations, and software. Data and products generated from Broader Impact activities, such as educational materials, participant information, tutorials and other web-based materials, as well as assessment results, should also be included in this section of the DMP.

### 2. Data Format

This section describes the format and media in which the data or products are stored (e.g., hardcopy notebook and/or instrument outputs, ASCII, html, jpeg or other formats). Where data are stored in unusual or not generally-accessible formats, the PI should explain how the data may be converted to a more accessible format or otherwise made available to interested parties. In general, solutions and remedies to providing data in an accessible format should be provided with minimal added cost.

### 3. Access to Data and Data Sharing Practices and Policies

“Access to data” refers to data made accessible without explicit request from the interested party, for example those posted on a website or made available to a public database. In this part of the DMP, the PI should describe plans, if any, for providing general access to data, including websites maintained by the PI’s research group, and direct contributions to public databases or software repositories (e.g., NMRShiftDB, the Protein Data Bank, Cambridge Crystallographic Data Centre, Inorganic Crystal Structure Database in Karlsruhe, Zeolite Structure Database, Github). For software or code developed as part of the project, a description of how users can access the code (e.g., licensing, open source) and specific details of the hosting, distribution and dissemination plans should be included, as well as the practice or policies regarding the release of data for access, for example whether data are posted before or after formal publication. Note as well any anticipated inclusion of the data in databases that mine the published literature (e.g., PubChem, NIST Chemistry Web

Book). Consider using the Digital Object Identifiers (DOI) assignment mechanism not just for journal articles, but for suitably-archived, publishable data sets. “Data sharing” refers to the release of data in response to a specific request from an interested party. This section also includes a description of policies for data sharing including, where applicable, provisions for protection of privacy, confidentiality, intellectual property, national security, or other rights or requirements. Discussion on the compliance with the NSF’s [Public Access Policy](#) is also encouraged.

### 4. Policies for Re-Use, Re-Distribution, and Production of Derivatives

Describe your policies regarding the use of data provided via general access or sharing. Practices for appropriate protection of privacy, confidentiality, security, intellectual property, and other rights should be communicated. The rights and obligations of those who access, use, and share your data with others should be defined. For example, if you plan to provide data and images on your website, will the website contain disclaimers, or conditions regarding the use of the data in other publications or products?

### 5. Archiving of Data

CHE-supported large research centers or other consortium programs may specify more stringent data storage, sharing and archiving procedures for research conducted under these programs. Any such more-stringent requirements will be specified in the program solicitation and award conditions.

## POST-AWARD MANAGEMENT

If an award is made, the PI must manage the data resulting from the project as described in the DMP presented in the original proposal, and should report these data-related activities in annual and final project reports<sup>6</sup>, and in Prior Result sections of through subsequent proposals to the NSF. Annual and final project reports are a critical mechanism for communication between the PI and the award’s managing Program Director.

<sup>6</sup> NSF guidance on Technical Reporting Requirements state that annual and final reports should describe actions taken during the reporting period to bring a proposal’s Data Management Plan to completion. See [NSF 16-040](#).

The NSF report format includes specific sections on the accomplishments and products of the research, including how the results have been disseminated to communities of interest a topic of importance in the DMP. Project reports should include specific information such as identifier or accession numbers for data sets, metadata and data annotation, citations of relevant publications<sup>7</sup> conference proceedings, details of software hosting, and other types of data sharing and dissemination, and updated information on project mechanisms for data storage, protection, and backup. CHE encourages investigators to use persistent identifiers (where these exist) as a long-lasting reference to a digital resource.

Final project reports should describe the implementation of the DMP and include any changes from the original DMP.

Note: Simply putting data in Supplementary Materials of a publication is not sufficient data management. The availability of the data should be advertised through a publicly accessible website and there should be adequate annotation provided, including what the data are and the parameters that were used to generate them to allow for reproducibility.

## FUTURE PROPOSALS

DMP implementation will also be considered during review of subsequent proposals. As described in the **PAPPG Part I Section II.C.2.d.iii**, the following information pertaining to past data management must be provided in the section ‘Results from Prior NSF Support:’

(e) Evidence of research products and their availability, including, but not limited to: data, publications, samples, physical collections, software, and models, as described in any Data Management Plan

## DATA MANAGEMENT RESOURCES

There are many resources available to PIs that provide assistance and information for planning and implementing a DMP. **Please note that inclusion of a particular resource in the list below is not intended as an endorsement by the NSF or the Division of Chemistry.**

Many university and college libraries provide resource guides or e-library consulting services to assist PIs in data management planning and best practices. These university data management groups can serve as a source of information for DMP topics such as data archiving and backup and open source distribution. For example:

Boston University Libraries – [Research Data Management](#)

UC San Diego Library – [Research Data Curation Program](#)

If you are unsure where to deposit your data, you might consider the use of online registries of research data repositories. See [re3data.org](http://re3data.org) for an extensive, though not exhaustive, list.

Professional societies will often also provide guidance for data achieving to the research community. The American Chemical Society has a position statement on [Ensuring Access to High-Quality Science](#).

Numerous non-governmental organizations offer resources and training for developing DMPs. These can be helpful, even if the target scientific discipline is not Chemistry. For example:

- [DataOne](#)
- [Software Carpentry](#)
- [DMPTool](#)
- [LTER](#)

## APPENDIX – BACKGROUND

Beginning in January 2011, NSF implemented a data management plan requirement for all proposals, which is described in the **Proposal & Award Policies & Procedures Guide (PAPPG) Part I Section II.C.2.j**. This requirement was created to aid in the dissemination, accessibility, and preservation of data generated by NSF-funded research. The goal of a DMP should be to provide clear, effective, and transparent implementation of the NSF policy on **Dissemination and Sharing of Research Results** as described in the **PAPPG Part II Chapter XI.D.4** and below.

<sup>7</sup> Publications from new awards resulting from proposals submitted after January 25, 2016 must be deposited in the NSF Public Access Repository (NSF-PAR). For more information, see [NSF's Public Access Initiative](#) and [FAQ for Public Access](#).

### Dissemination and Sharing of Research Results

- F. Investigators are expected to promptly prepare and submit for publication, with authorship that accurately reflects the contributions of those involved, all significant findings from work conducted under NSF grants. Grantees are expected to permit and encourage such publication by those actually performing that work, unless a grantee intends to publish or disseminate such findings itself.
- G. Investigators are expected to share with other researchers, at no more than incremental cost and within a reasonable time, the primary data, samples, physical collections and other supporting materials created or gathered in the course of work under NSF grants. Grantees are expected to encourage and facilitate such sharing. Privileged or confidential information should be released only in a form that protects the privacy of individuals and subjects involved. General adjustments and, where essential, exceptions to this sharing expectation may be specified by the funding NSF Program or Division/Office for a particular field or discipline to safeguard the rights of individuals and subjects, the validity of results, or the integrity of collections or to accommodate the legitimate interest of investigators. A grantee or investigator also may request a particular adjustment or exception from the cognizant NSF Program Officer.
- H. Investigators and grantees are encouraged to share software and inventions created under the grant or otherwise make them or their products widely available and usable.
- I. NSF normally allows grantees to retain principal legal rights to intellectual property developed under NSF grants to provide incentives for development and dissemination of inventions, software and publications that can enhance their usefulness, accessibility and upkeep. Such incentives do not, however, reduce the responsibility that investigators and organizations have as members of the scientific and engineering community, to make results, data and collections available to other researchers.
- J. NSF program management will implement these policies for dissemination and sharing of research results, in a way appropriate to field and circumstances, through the proposal review process; through award negotiations and conditions; and through appropriate support and incentives for data cleanup, documentation, dissemination, storage and the like.
- K. Each NSF grant contains, as part of the grant terms and conditions, an article implementing dissemination and sharing of research results.

## NEWLY REVISED PROGRAM DESCRIPTIONS

### CHEMICAL CATALYSIS (CAT)

The Chemical Catalysis Program supports experimental and computational research directed towards the fundamental understanding of the chemistry of catalytic processes. The CAT Program accepts proposals on catalytic approaches, which facilitate, direct, and accelerate efficient chemical transformations. The program scope includes the design and synthesis of catalytic species on the molecular, supramolecular, and nanometer scales as well as mechanistic studies primarily focused on discovery, development, or improvement of homogeneous and heterogeneous catalytic processes. The CAT Program also considers (but is not limited to) the following: polymerization catalysis, single site catalysis, organocatalysis, inorganic, organometallic, and photoredox catalysis, electrocatalysis, and biologically-inspired catalysis. Applications of modeling, theory, and simulation to catalytic processes are also relevant. Fundamental studies of energy-related catalytic processes (such as in water splitting and fuel cells) and photocatalysis (such as in solar energy conversion) are welcome in the CAT Program.

Submissions that address national needs for sustainability are particularly encouraged. Examples of sustainable chemistry appropriate for the Chemical Catalysis Program include, but are not limited to: the design, preparation and reactivity studies associated with new catalysts and catalytic processes that will replace rare, and/or toxic compounds with earth-abundant and benign alternatives and advanced catalytic methods for the reduction of dinitrogen to ammonia that will permit reductions in the energy requirements and greenhouse gas emissions for fertilizer production.

The CAT Program does not support applied catalysis research focusing on engineering aspects of catalysis such as scale-up, processing, transport dynamics, and long-term stability. Researchers contemplating proposals in these areas are directed to the NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET). Researchers focused on enzymatic or cellular catalysis should consult the Chemistry of Life Processes (CLP) Program. Catalysis research with immediate objectives in the synthesis of complex natural products using established catalysts should be submitted to the Chemical Synthesis (SYN) Program. Finally, research primarily targeted at catalytic reaction mechanisms using known catalysts are most appropriate for submission to the Chemical Structures, Dynamics and Mechanisms–B (CSDMA-B) Program.

## CHEMICAL THEORY, MODELS & COMPUTATIONAL METHODS (CTMC)

The Chemical Theory, Models, and Computational Methods Program supports the discovery and development of theoretical and computational methods or models to address a range of chemical challenges, with emphasis on emerging areas of chemical research. Proposals that focus on established theoretical or computational approaches should involve innovations that substantially broaden their applicability. Areas of interest include, but are not limited to, electronics structure, quantum reaction dynamics, theoretical/computational spectroscopy, statistical mechanics, molecular dynamics and simulation, and modeling techniques for isolated molecular systems and systems in complex environments. Areas of application span the full range of chemical systems from single molecules to mesoscopic aggregates. Proposals that develop approaches to bridge multiple spatial or temporal scales are welcome. Despite the diverse application areas, the goal of the program is to support the development of new theoretical and computational methodologies that are broadly applicable to a range of challenging chemical problems. The CTMC Program is interested in fundamental areas of chemical research that are difficult or impossible to address using current synthetic, experimental, and/or computational methodologies.

We encourage proposals that address emerging areas in theoretical and computational chemistry, including proposals that involve novel approaches based on machine learning or other data-enabled methods with broad applicability to significant chemical problems. We also encourage proposals on quantum information science (QIS) that either focus on applying QIS concepts to theoretical and computational chemistry or on developing quantum algorithms for chemical systems.

The CTMC Program encourages the integration of innovative software development with methodological and algorithmic development, especially computational approaches that allow efficient utilization of emerging computer architectures. Such proposals may be submitted to the CTMC Program either directly or through the Computational and Data Science and Engineering (CDS&E) funding opportunity: [https://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=504813](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504813). Note: Relevant proposals should have a title starting with “CDS&E:” to be distinguished from other CTMC proposals.

Proposals that utilize established theoretical and modeling approaches to solve problems in chemistry without significant theoretical or methodological development, or that focus on the development of biology or materials design may be more appropriate for other programs in either the Chemistry Division or in other NSF Divisions or Directorates.

## ENVIRONMENTAL CHEMICAL SCIENCES (ECS)

The Environmental Chemical Sciences (ECS) Program supports experimental and computational research on the fundamental chemistry of processes in the environment. Recognizing the intrinsic complexity and heterogeneity of environmental systems, projects develop and utilize advanced experimental, modeling and simulation approaches to discover, explain, and predict environmental phenomena. Topics may include, but are not limited to: processes occurring at environmental interfaces and the chemical behavior and transformation under a variety of naturally occurring environmental conditions.

Submissions that address national needs for sustainability are particularly encouraged. Examples of sustainable chemistry appropriate for the ECS Program include, but are not limited to: proposals that consider the nexus of food, energy, and water sustainability especially as related to nitrogen and phosphorus cycling.

Field measurements and instrument development in support of environmental measurements are not supported. Programs in other NSF Directorates and other Federal Agencies address aspects such as field studies, large-scale models of the environment, toxicity studies, industrial processes, remediation methods, and the behavior and fate of nanoparticles in the environment.

## CHEMICAL STRUCTURE, DYNAMICS & MECHANISMS (CSDM)

The Chemical Structure, Dynamics and Mechanisms (CSDM) Programs support chemistry research that has strong implications for advancing the foundational knowledge of chemical systems. The Program supports research on the nature of chemical structure, structure-property studies, thermodynamics and kinetics, and mechanisms. The CSDM Program is divided into two sub-programs, CSDM-A and CSDM-B. The research supported by the two programs is distinguished in terms of whether their goal is to challenge thinking about physical phenomena in chemical systems through the development of innovative experimental approaches and new conceptual models (CSDM-A) or to use existing experimental methods and current conceptual frameworks to understand and describe physical processes in molecules and materials that are becoming increasingly relevant in modern applications (CSDM-B). Projects supported by CSDM-A typically involve in-depth analysis of experimental data at the quantum- or statistical-mechanical level, often with an outcome being the modification or updating of the theoretical model. Projects supported by CSDM-B also rely on theory to interpret structure-function relationships, but tend to focus on the consequence of structure (or changes in structure) on reactivity and other behaviors.

Projects involving nanochemistry or biologically-relevant systems should consult the Macromolecular, Supramolecular and Nanochemistry (MSN) or Chemistry of Life Processes (CLP) Programs, respectively. Proposals for projects whose primary goal is the development of an entirely new instrumental technique, or enhanced performance or understanding of an existing technique may be more appropriate for the Chemical Measurement and Imaging (CMI) Program. In general, research focused on solid-state chemical processes are not supported by CSDM. Investigators interested in this area should consult with the Solid State Materials Chemistry (SSMC) Program in the Division of Materials Research (DMR). Projects for which the primary goal is the development of a practical device are not supported by the CSDM-A and CSDM-B Programs and should be submitted to an appropriate program in the Engineering Directorate.

The following Program Descriptions are intended to guide the proposer to the most appropriate sub-program for her/his research.

### THE CHEMICAL STRUCTURE, DYNAMICS AND MECHANISMS-A (CSDM-A)

The Chemical Structure, Dynamics and Mechanisms-A (CSDM-A) Program supports experimental and applied computational research directed at increasing our fundamental understanding of the physical properties of chemical systems at the quantum and/or statistical mechanical level. Projects of interest to CSDM-A rely heavily on the advancement of sophisticated experimental techniques, such as: state-selective methods, time and frequency domain spectroscopies, microscopies, single-molecule methods, scattering and diffraction approaches, and surface characterization techniques. The program is interested in projects where the development of novel methods enables the physical behavior of chemical systems to be viewed in new ways, or in ways that challenge current paradigms. Chemical systems studied range in complexity and include isolated molecules and ions, liquids, clusters, surfaces, and interfaces. The CSDM-A Program also supports applied computational chemistry activities that demonstrate strong synergy with experiment.

Submissions that address national needs are particularly encouraged. These may include, but are not limited to: quantum chemistry where the focus is on the application of quantum mechanics in physical models and experiments of chemical systems.

### THE CHEMICAL STRUCTURE, DYNAMICS AND MECHANISMS-B (CSDM-B)

The Chemical Structure, Dynamics and Mechanisms-B (CSDM-B) Program supports mechanistic studies of various chemical processes and chemical property studies. CSDM-B proposals generally utilize existing experimental techniques as opposed to developing new ones so that the work can focus on new understanding of molecular properties. The CSDM B program supports research on the consequences of molecular structure on chemical properties and mechanisms. Topics of interests to CSDM-B include (but are not limited to): mechanistic studies of chemical reactions, and energy- or materials-related processes, the chemistry of reactive intermediates, and the development of molecules with novel chemical properties. Projects supported in the CSDM B program are diverse, ranging from traditional mechanistic studies, chromophore development for advance imaging and solar applications, to studies relevant to the development of flow batteries and molecular qubits. Projects in the CSDM B program often involve significant synthetic efforts in order to vary the chemical structures.

Submissions that address national needs such as sustainability, brain research, quantum information science, and data are encouraged.

## MACROMOLECULAR, SUPRAMOLECULAR & NANOCHEMISTRY (MSN)

The Macromolecular, Supramolecular and Nanochemistry (MSN) Program focuses on basic research that addresses fundamental questions and advances knowledge regarding the chemistry of macromolecular, supramolecular, and nanoscopic structures. Research of interest to this program will explore novel chemistry concepts including, but not limited to: synthesis of macromolecular, supramolecular and nanoscopic structures; surface functionalization methodologies; surface monolayer chemistry; and template-directed synthesis; inter- and intra-molecular interactions that give rise to macromolecular, supramolecular or nanoparticulate self-assembly into discrete structures; and chemical dynamics that are responsible for spatial organization in discrete organic, inorganic, or hybrid systems (excluding extended solids). Also included are advanced experimental or computational methods to delineate or to predict the chemical structure, unique chemical and physicochemical properties, and chemical reactivity that result from macromolecular, supramolecular, and nanoscopic structures, including systems that exhibit quantum confinement and other non-classical effects. Projects which demonstrate synergy between experiment and theory are of special interest.

Submissions that advance MSN chemistry knowledge important for addressing national needs in sustainability are strongly encouraged. Examples include, but are not limited to: transformative approaches to efficient and inexpensive synthesis using renewable feedstocks or earth abundant elements; and innovative research that enhances the understanding of efficient use and recycling of critical elements or the conversion of energy from renewable sources.

Proposals for which the primary focus is on single molecules, extended solids (including metal organic frameworks), materials research, fate of nanoparticles in the environment, device properties, engineering, biological properties (including toxicity), drug delivery, or selection or genetic engineering of enzymes are not of interest in the MSN Program. Investigators interested in these areas are encouraged to approach other, more closely aligned programs such as those in the Divisions of Materials Research (DMR), Physics (PHY), and Chemical, Bioengineering, Environmental, and Transport Systems (CBET).

## CHEMICAL SYNTHESIS (SYN)

The Chemical Synthesis Program supports experimental and computational research on the development of new and efficient synthetic methodologies and on the synthesis of complex and/or challenging chemical structures. Typical synthetic targets include novel structures (including natural products and biomolecules), molecules and structures displaying unique properties, or substances that provide pathways to discover and elucidate new phenomena. Examples of supported research areas include the development of innovative reagents, discovery of new synthetic methods, and synthesis of novel organic, organometallic, and inorganic structures. Research in this program will generate fundamental new knowledge of chemical synthesis, but also enable new discoveries and the development of transformative technologies in related fields.

Submissions that address national needs for sustainability are encouraged. Examples include, but are not limited to: the development of new synthetic methods using earth-abundant and inexpensive chemicals, fundamental studies that improve our understanding of rare earth elements; the conversion of non-petroleum based resources into useful building blocks; and new environmentally-friendly chemical syntheses that improve on current practice by requiring less energy, fresh water, reagents, and/or organic solvents.

The Chemical Synthesis Program does not support projects where the main objectives are to study the properties of target systems, even though they may contain a large synthetic component. Proposed studies of this nature may be directed to the Chemical Structure, Dynamics, and Mechanism-B (CSDM-B) Program. Investigators interested in developing novel synthetic approaches to macromolecular, supramolecular and nanoscale chemical structures should consult the Macromolecular, Supramolecular and Nanochemistry (MSN) Program. Projects developing syntheses of extended solids should consult the Division of Materials Research (DMR). Proposals that have a major focus on the design of new catalysts and study of catalytic reactions should be submitted to the Chemical Catalysis (CAT) Program.

## CHEMISTRY OF LIFE PROCESSES (CLP)

The Chemistry of Life Processes (CLP) Program supports fundamental experimental and computational studies of molecules and/or systems at the interface of chemistry and biology. Such studies would promote the fundamental understanding of

the molecular underpinnings of life processes. The proposed research should focus on the chemical aspects of the project. The Program supports studies that investigate how molecular structure, dynamics and interactions, as well as reaction thermodynamics and mechanisms are integrated with the chemistry performed by the biological systems.

Research projects typically employ experimental, theoretical, computational or integrated approaches to investigate biological systems such as, but not limited to, proteins, nucleic acids, carbohydrates or lipids. Projects that use or reveal novel chemistries, in advancing the understanding of biological function, are particularly welcome. Chemical methods development is acceptable when such methods are applied in addressing specific biological questions.

Submissions that address national needs are encouraged. These may include, but are not limited to: proposals that address the function of the brain as well as proposals that examine the “rules of life”. Other topics of interest include: the development and application of bio-orthogonal chemistry for probing cellular function; the quantitative understanding of thermodynamics as applied to a cellular system; biomolecular design and synthesis aimed at understanding biological function; and the use of theory, computation, modeling and simulation as applied to the chemical aspects of biological systems.

Note: The CLP Program is interested in understanding function rather than malfunction or dysfunction. Projects that are disease-related, or that have drug discovery/design/development goals are not appropriate for review in the CLP Program. PIs uncertain of the fit of their proposal are encouraged to contact a CLP Program Officer.

## CHEMICAL MEASUREMENT AND IMAGING (CMI)

The Chemical Measurement and Imaging Program supports research focusing on chemically-relevant measurement science and imaging, targeting both improved understanding of new and existing methods and development of innovative approaches and instruments. Research areas include, but are not limited to: sampling and separation science; electroanalytical chemistry; spectrometry; and frequency- and time-domain spectroscopy. Development of new chemical imaging and measurement tools probing chemical properties and processes are supported. Innovations enabling the monitoring and imaging of chemical and electronic processes across a wide range of time and length scales are also relevant. New approaches to data analysis and interpretation (including chemometrics) are encouraged. Proposals addressing established techniques must seek improved understanding and/or innovative approaches to substantially broaden applicability. Sensor-related proposals should address new approaches to chemical sensing, with prospects for broad utility and significant enhancement of current capabilities.

Submissions that address national needs are encouraged. Such proposals may include, but are not limited to new measurement and imaging approaches that improve on current separation science by requiring less energy or generating less waste, on understanding the brain and its functions, and on harnessing the power of chemical data.

Topics also considered by CMI include the development of new instrumentation enabling chemical measurements likely to be of wide interest and utility to the chemistry research community. These proposals should include the words “Instrument Development:” at the beginning of the title, and include, in the Project Description, consideration of a development timeline, potential utility, and prospects for the extension of the technique to other uses or fields, should it prove viable.

Industrial partnerships are encouraged through the Grant Opportunities for Academic Liaison with Industry (GOALI) mechanism ([https://www.nsf.gov/pubs/policydocs/pappg17\\_1/pappg\\_2.jsp#IIE4](https://www.nsf.gov/pubs/policydocs/pappg17_1/pappg_2.jsp#IIE4)) as means enhancing use by the greater community, but concepts nearing commercialization are better fits to Small Business Innovation Research (SBIR) or Small Business Technology Transfer (STTR) Programs.

Proposals integrating innovative computational approaches with CMI-relevant research, such as those enabling efficient and effective data acquisition and analysis, are encouraged and should be submitted to the CMI Program through the Computational and Data Science and Engineering (CDS&E) funding opportunity ([https://www.nsf.gov/funding/pgm\\_summ.jsp?pims\\_id=504813](https://www.nsf.gov/funding/pgm_summ.jsp?pims_id=504813)).

The CMI Program does not encourage proposals addressing: the development of techniques for topological/morphological imaging; research based on known sensing mechanisms, such as probe synthesis or assembly of array-type devices; or engineering aspects of membrane separations, microfluidics, and/or “lab-on-a-chip” device design, technology, and application. Proposals on the design and synthesis of novel molecular probes for sensing or contrast agents may be more suitable for the CSDM-B Program. Proposals for optimizing and/or utilizing established methods for specific applications should be directed to programs focused on the application. Proposals addressing innovations with anticipated utility primarily in other communities (e.g., biology or materials) are also not encouraged. Proposals with large equipment requests (over \$150,000) may be better suited to the Major Research Instrumentation (MRI) Program.

## CENTERS FOR CHEMICAL INNOVATION (CCI)

The Centers for Chemical Innovation (CCI) Program supports research centers focused on major, long-term fundamental chemical research challenges. CCIs that address these challenges are expected to produce transformative research, lead to innovation in the discipline, and attract broad scientific and public interest. CCIs are agile structures that respond rapidly to emerging opportunities through enhanced collaborations. CCIs integrate research, innovation, education, broadening participation, and informal science communication.

The FY 2018 Phase I CCI competition is open to projects in all fields supported by the Division of Chemistry, and must have focus and the potential for transformative impact in chemistry. NSF Chemistry particularly encourages projects in Data-Driven Discovery Science in Chemistry (*D3SC*).

The CCI Program is a two-phase program. Both phases are described in *NSF 17-564*. Phase I CCIs receive significant resources to develop the science, management and broader impacts of a major research center before requesting Phase II funding. Satisfactory progress in Phase I is required for Phase II applications; Phase I proposals funded in FY 2018 will seek Phase II funding in FY 2021. This solicitation also covers the renewal application of the Phase II CCI initiated in FY 2013: CAICE, led by the University of California San Diego.

### Phase I due dates:

- ▮ Preliminary Proposals are due by September 12, 2017
- ▮ Full Proposals, by invitation only, are due by March 06, 2018

Interested investigators are encouraged to discuss their ideas with a CCI Program Officer. Contact information and more information can be found in the document below: [https://www.nsf.gov/publications/pub\\_summ.jsp?ods\\_key=nsf17564](https://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf17564)

## WORKSHOP REPORTS

Recently posted workshop reports are available on the Chemistry website. CHE is deeply indebted to the workshop organizers, steering committees, and participants – thank you all for your efforts to provide valuable perspectives for consideration by the entire chemistry community.

Measuring the Brain: From the Synapse to Thought was held on October 12-13, 2016. Report: <https://beckman.illinois.edu/Content/uploads/files/groups/neurotech-memory-cognition/measuring-the-brain-from-synapse-to-thought-nsf-10-2016.pdf>.

Appendices: <https://beckman.illinois.edu/Content/uploads/files/groups/neurotech-memory-cognition/nsf-brain-appendices-10-2016.pdf>

Mid-Scale Instrumentation Workshop: Regional Facilities to Address Grand Challenges in Chemistry held on September 29-30, 2016. [http://nsfmidscale.chem.wisc.edu/sites/nsfmidscale.chem.wisc.edu/files/report/MSIregionalcenters\\_FINALworkshopreport\\_5\\_1\\_17.pdf](http://nsfmidscale.chem.wisc.edu/sites/nsfmidscale.chem.wisc.edu/files/report/MSIregionalcenters_FINALworkshopreport_5_1_17.pdf)

Mid-Scale Instrument Development Workshop was held on November 6-8, 2016. <https://advanceddiagnostics.nd.edu/opportunities/nsf-workshop/>

Quantum Information and Computation for Chemistry Workshop held on November 13-14, 2016. <https://arxiv.org/pdf/1706.05413.pdf>

## MOLECULAR SCIENCES SOFTWARE INSTITUTE (MOISSI)

The Molecular Sciences Software Institute (MolSSI) is a new initiative supported by the National Science Foundation to serve as a nexus for science, education, and cooperation for the community of computational molecular scientists — a broad field that includes biomolecular simulation, quantum chemistry, and materials science. The MolSSI's goal is to enable molecular scientists to tackle problems that are orders of magnitude larger and more complex than those currently within our grasp.

The MolSSI will engage a team of Software Scientists (molecular scientists, computer scientists, and applied mathematicians with software engineering expertise) to develop open-source software infrastructure for use across the spectrum of community molecular science codes. The MolSSI supports a series of community-led workshops targeting software-related challenges relevant to the computational molecular sciences, as well as Software Summer Schools focused on undergraduate and graduate students across the United States.

The MolSSI will also recognize advanced graduate students and postdocs through a number of prestigious Software Fellowships that include generous financial support, specialized training in state-of-the-art software design principles and tools, and involvement in the Institute's outreach and educational efforts. Under the guidance of the MolSSI's Software Scientists, the Software Fellows will develop open-source software infrastructure for broad use across the computational molecular sciences. The Software Fellowships will be awarded using a two-phase structure, providing up to two years of support. The first Phase-I Software Fellows were announced in April at the American Chemical Society meeting in San Francisco, and the next window for applications will close October 1.

Learn more about how the MolSSI can serve you at our website: [molssi.org](http://molssi.org)

## AMERICAN CHEMICAL SOCIETY (ACS) NATIONAL MEETING 254<sup>TH</sup> AMERICAN CHEMICAL SOCIETY NATIONAL MEETING AND EXPOSITION

The Division of Chemistry will participate in this year's 254th American Chemical Society (ACS) National Meeting and Exposition in Washington, DC on August 20-24, 2017.

ACS Meeting website: <https://www.acs.org/content/acs/en/meetings/fall-2017.html>

Please mark your calendar with the following days and times to find NSF Staff at the following presentations.

### **Inorganic Chemistry Division Poster Session**

Sunday, August 20, 2017 from 7:00 — 9:00 P.M.

Walter E. Washington Convention Center

Come and meet NSF Staff at the Inorganic Chemistry Poster Session.

### **Please stop by the CCI oral presentations and poster sessions:**

A symposium celebrating the contributions CENTC has made to catalysis will be held during the 254th ACS National Meeting in Washington DC. The symposium "Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration" is part of the Inorganic Division programming and assembles a diverse group of 34 CENTC alumni, advisory board members and investigators for oral presentations scheduled in morning and afternoon sessions on Monday and Tuesday, August 21 and 22. There are also poster sessions associated with the symposium where 47 current CENTC students, postdocs, and alumni will present their work on Sunday and Tuesday evenings, August 20 and 22.

### Center for Enabling New Technologies through Catalysis: Transforming Catalysis through Collaboration

#### Oral Presentations:

Monday, August 21, 8:30 – 12:15 & 1:30 – 5:10  
Tuesday, August 22, 8:30 – 12:00 & 1:30 – 5:20  
Grand Ballroom Central, Renaissance Washington, DC  
Downtown

#### Posters:

Sunday, August 20 & Tuesday, August 22, 5:30  
Hall D, Walter E. Washington Convention Center

Monday, August 21, 2017 from 8:00 — 10:00 P.M.  
Walter E. Washington Convention Center

Come meet NSF Staff at the Sci-Mix Poster Session.

Tuesday, August 22, 2017 from 9:00 — 12:00 P.M.  
Walter E. Washington Convention Center  
The World of Funding Opportunities in Chemistry  
Poster Session

This poster session is designed to introduce the chemical community to the diverse research support options available, ranging from the more traditional support provided by federal agencies to that available from industry, government labs, private foundations, and international groups.

Tuesday, August 22, 2017 from 1:00 — 3:00 P.M.  
Walter E. Washington Convention Center  
Federal Funders Town Hall Meeting

Come learn about agency priorities, initiatives, programs, and how to participate at the Federal Funders Town Hall.

#### Below is a list of some of the Federal Funders attending:

National Science Foundation  
(NSF CHE, DMR, CBET, and EHR)  
Department of Energy (DOE BES)  
National Institutes of Health (NIH and NIGMS)  
Air Force Office of Scientific Research (AFOSR)  
The Office of Naval Research (ONR)

Tuesday, August 22, 2017 from 3:00 — 5:00 P.M.  
(Sign-Up from 10:00 – 12:00 PM.)  
Walter E. Washington Convention Center  
Federal Funders Town Hall Meeting Speed  
Coaching Session

Come join speed coaching and receive a one-on-one interaction with a federal Program Officer to discuss research, education, and outreach activities. All are welcome – Registration not required! For additional information, email:  
[cheminfo@nsf.gov](mailto:cheminfo@nsf.gov)

*\*please check back on our website ([www.nsf.gov/chem](http://www.nsf.gov/chem)), for meeting locations.*

The NSF Staff is looking forward to another successful and productive meeting and exposition!

Website: [molssi.org](http://molssi.org)

## 2017 CHEMISTRY CAREER AWARDEES

Congratulations to the NSF/Chemistry 2017 CAREER Awardees. The faculty Early Career Development (CAREER) Program is a Foundation-wide activity that offers the NSF's most prestigious awards in support of junior faculty who exemplify the role of teacher-scholars through outstanding research, excellent education and the integration of education and research within the context of the mission of their organizations. Such activities should build a firm foundation for a lifetime of leadership in integrating education and research.

### We hereby recognize the NSF/CHE CAREER Awardees, Class of 2017!



**John Anderson**  
University of Chicago  
Award Number: 1654144  
Title: CAREER:  
*Probing Catalytic O-O Bond  
Formation with  
Pseudo-Tetrahedral  
Terminal Oxo Complexes.*



**Alfredo Angeles-Boza**  
Deputy Division Director  
University of Connecticut  
Award Number: 1652606  
Title: CAREER: SusChEM: Heavy  
Atom Isotope Effects in Carbon  
Dioxide Fixation Catalysis:  
Fundamental Understanding and  
Catalyst Discovery.



**Andrew Ault**  
University of Michigan  
Award Number: 1654149  
Title: CAREER: Molecular Studies  
of Phase Separations and Internal  
Structure in Individual Particles.



**Christian Bleiholder**  
Florida State University  
Award Number: 1654608  
Title: CAREER: Ion Mobility  
Spectrometry - Mass  
Spectrometry for de novo  
Protein Structure Elucidation.



**Marco Caricato**  
University of Kansas  
Center for Research Inc.  
Award Number: 1650942  
Title: CAREER: First Principles  
Evaluation of Optical Activity  
in Solids.



**Bradley Carrow**  
Princeton University  
**Award Number:** 1654664  
**Title:** CAREER: Enabling Sustainable Polymer Synthesis through Design of New Catalysts.



**Louise Charkoudian**  
Haverford College  
**Award Number:** 1652424  
**Title:** CAREER: Accessing Chemical Diversity through the Characterization and Redesign of Natural Product Syntheses.



**Scott Daly**  
University of Iowa  
**Award Number:** 1650894  
**Title:** CAREER: SusChEM: Coupling Earth-Abundant Metal-Ligand Cooperativity with Redox Non-Innocent Ligands for Electrochemical Carbon Dioxide Reduction.



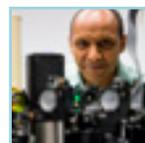
**Tianning Diao**  
New York University  
**Award Number:** 1654483  
**Title:** CAREER: Bimolecular Mechanisms for Nickel-Mediated Bond Formation.



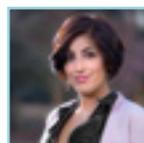
**Francisco Fernandez-Lima**  
Florida International University  
**Award Number:** 1654274  
**Title:** *Development of Gas-phase, Post-ionization Structural Tools for the Study of DNA-protein Complexes.*



**Yisong Guo**  
Carnegie-Mellon University  
**Award Number:** 1654060  
**Title:** CAREER: Kinetic and Spectroscopic Studies of Catalytically Versatile Non-heme Mononuclear Iron Enzymes.



**Terefe Habteyes**  
University of New Mexico  
**Award Number:** 1651478  
**Title:** CAREER: Near-Field Imaging for Nanoscale Visualization of Exciton-Plasmon Energy Transfer.



**Parastoo Hashemi**  
University of South Carolina at Columbia  
**Award Number:** 1654111  
**Title:** CAREER: The fundamental principles of modified carbon fiber microelectrodes as speciation sensors.



**Yilin Hu**  
University of California, Irvine  
**Award Number:** 1651398  
**Title:** CAREER: CO<sub>2</sub> activation by nitrogenase Fe proteins.



**Stefan Kilyanek**  
University of Arkansas  
**Award Number:** 1654553  
**Title:** CAREER: SusChEM : Electrochemically Driven Deoxydehydration of Polyols.



**Bo Li**  
University of North Carolina at Chapel Hill  
**Award Number:** 1654678  
**Title:** CAREER: Combining Chemistry with Bioinformatics to Discover Novel Transformations of Nonproteinogenic Amino Acids.



**Alexander Lippert**  
Southern Methodist University  
**Award Number:** 1653474  
**Title:** CAREER: Triggered Energy Transfer Chemiluminescence for In Vivo Imaging.



**Peng Liu**  
University of Pittsburgh  
**Award Number:** 1654122  
**Title:** CAREER: Computational Studies of Transition Metal Catalyzed Reactions in Organic Synthesis.



**Rob Macfarlane**  
Massachusetts Institute of Technology  
**Award Number:** 1653289  
**Title:** CAREER: Nanocomposite Structure Control via Nanoparticle Self-Assembly.



**Thomas Markland**  
Stanford University  
**Award Number:** 1652960  
**Title:** CAREER: Investigating the structure and dynamics of proton defects in heterogeneous environments with accelerated quantum simulations.



**Ellen Matson**  
University of Rochester  
**Award Number:** 1653195  
**Title:** CAREER: Synthesis, Characterization and Reactivity of Iron-Functionalized Polyoxovanadate-Alkoxide Clusters for the Activation of Small Molecules.



**Emily McLaurin**  
Kansas State University  
**Award Number:** 1654793  
**Title:** CAREER: Microwave-Assisted Ionic Liquid Etching of Colloidal III-V Semiconductor Nanocrystals.



**Bradley Merner**  
Auburn University  
**Award Number:** 1654691  
**Title:** CAREER: Functionalized Bent para-Phenylenes: New Strategies and Tools for the Synthesis of Carbon Nanotubes.



**Justin Mohr**  
University of Illinois at Chicago  
**Award Number:** 1654490  
**Title:** CAREER: Novel Methods for Regio-, Stereo-, and Chemo-selectivity Remote to Functional Groups.



**Gary Moore**  
Arizona State University  
**Award Number:** 1653982  
**Title:** CAREER: SUNCROPS (Solar-Fuels Using Nanoscale Catalysts Reacting on Polymer-modified Surfaces).



**David Nagib**  
Ohio State University  
**Award Number:** 1654656  
**Title:** CAREER: SusChEM: Anomeric Activation Strategy for Catalytic, Ketyl Radical Reactivity.



**Timothy Newhouse**  
Yale University  
**Award Number:** 1653793  
**Title:** CAREER: Palladium-Catalyzed Dehydrogenation of Carbonyl Compounds.



**Alexis Ostrowski**  
Bowling Green State University  
**Award Number:** 1653892  
**Title:** CAREER: Controlling mechanical properties of materials using photoactive metal coordination bonds.



**Michele Pavanello**  
Rutgers University  
**Award Number:** 1553993  
**Title:** CAREER: CDS&E: Nonlocal and Periodic Density Embedding.



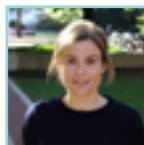
**Dmitry Peryshkov**  
University of South Carolina at Columbia  
**Award Number:** 1654301  
**Title:** CAREER: Carborane Cluster Architectures Featuring Multiple Metal-Boron Interactions.



**Sean Roberts**  
University of Texas at Austin  
**Award Number:** 1654404  
**Title:** CAREER: Tracking Charge and Energy Transfer at Buried Organic Interfaces.



**David Sarlah**  
University of Illinois at Urbana-Champaign  
**Award Number:** 1654110  
**Title:** CAREER: New Dearomative Methods and Strategies for Organic Synthesis.



**Corinna Schindler**  
University of Michigan, Ann Arbor  
**Award Number:** 1654223  
**Title:** CAREER: Enabling New Methodologies for the Synthesis of Polycyclic, Complex Molecules.



**Scott Shaw**  
University of Iowa  
**Award Number:** 1651381  
**Title:** CAREER: Crossing and Controlling the Bulk to Interface Transition: Chemical Profiles of Fluids Near Surfaces.



**Yujie Sun**  
Utah State University  
**Award Number:** 1653978  
**Title:** CAREER: SusChEM: Electrochemical Valorization of Biomass Intermediates via 1st-Row Transition Metal Electrocatalysts.



**Benjamin Swarts**  
Central Michigan University  
**Award Number:** 1654408  
**Title:** CAREER: Chemical Tools for Understanding the Mycomembrane of the Corynebacterineae.



**Michal Szostak**  
Rutgers University  
**Award Number:** 1650766  
**Title:** CAREER: Cross-Coupling via Amide Bond Cleavage: Development of Novel Synthetic Catalytic Methodology.



**Ryan Trovitch**  
Arizona State University  
**Award Number:** 1651686  
**Title:** CAREER: SusChEM: Development of Manganese Hydrosilylation Catalysts for Silicone Curing.



**Sergey Varganov**  
Board of Regents, NSHE, obo University of Nevada, Reno  
**Award Number:** 1654547  
**Title:** CAREER: Theoretical and computational methods for spin-forbidden processes in complex systems.



**Hailiang Wang**  
Yale University  
**Award Number:** 1651717  
**Title:** CAREER: Heterogeneous Molecular Catalysts for Electrochemical CO<sub>2</sub> Reduction.



**Davita Watkins**  
University of Mississippi  
**Award Number:** 1652094  
**Title:** CAREER: Elucidating the role of sigma-hole interactions in advanced functional materials



**Timothy Wenczewicz**  
Washington University  
**Award Number:** 1654611  
**Title:** CAREER: Siderophore Chemistry in Pathogenic Bacteria.



**Adam Willard**  
Massachusetts Institute of Technology  
**Award Number:** 1654415  
**Title:** CAREER: Characterizing Water's Response to Hydrophilic Surfaces.



**Xiaohu Xia**  
Michigan Technological University  
**Award Number:** 1651307  
**Title:** CAREER: Engineering Bimetallic Nanostructures as Peroxidase Mimics for Diagnostic Applications.



**Ruoxue Yan**  
University of California, Riverside  
**Award Number:** 1654794  
**Title:** CAREER: Development of Novel-scheme Nano-optical Chemical Imaging Spectroscopy.



**Ding-Shyue Yang**  
University of Houston  
**Award Number:** 1653903  
**Title:** CAREER: Visualizing Structures and Ultrafast Dynamics of Heterogeneous Interfaces Using Time-Resolved Electron Imaging.



**Joel Yuen-Zhou**  
University of California, San Diego  
**Award Number:** 1654732  
**Title:** CAREER: Molecular polaritons: new opportunities for spectroscopy and control of charge and energy transport.

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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)		

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**  
National Science Foundation  
4201 Wilson Boulevard, Arlington, Virginia 22230

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