

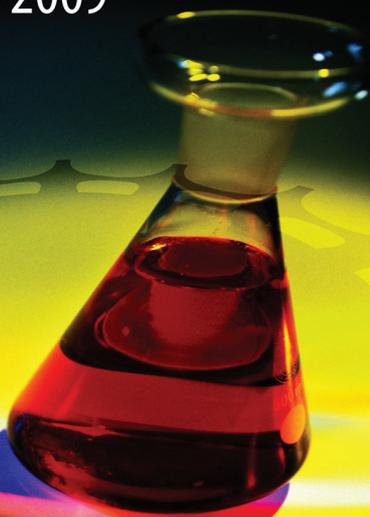
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United States of America
National Science Foundation



**DIVISION
OF
CHEMISTRY**

Realignment of the
Division of Chemistry Programs
2009



The mission of the NSF Division of Chemistry is to support innovative research in chemical sciences, integrated with education, through strategic investment in developing a globally engaged U.S. chemistry workforce reflecting the diversity of America.

Dear Colleague,

Greetings and welcome to National Science Foundation (NSF) Division of Chemistry. In April 2008 the division published its 2008-2012 Strategic Directions. One of the eight critical issues identified in the report was *Updating the Division of Chemistry Structure*. The goal is to structure the Division to best anticipate and respond to scientific needs and to achieve transformative research in chemistry. The Strategic Directions document and its history are available at http://www.nsf.gov/mps/che/CHE_StrategicDirections.pdf.

With the implementation of the Division realignment, we have established eight new programs while retaining the family of programs housed in Integrative Chemistry Activities. Descriptions of the programs are provided in this brochure.

I look forward to hearing your thoughts and comments about the realignment of the Division's programs. If you cannot speak with me or a Program Director in person, please submit your comments to chemplans@nsf.gov.

Sincerely,

A handwritten signature in black ink, appearing to read "Luis Echegoyen". The signature is fluid and cursive, with a long horizontal stroke extending to the right.

Luis Echegoyen, Director
Division of Chemistry
National Science Foundation
(703) 292-4960
lechegoy@nsf.gov



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These programs accept individual and collaborative proposals that are responsive to the NSF Grant Proposal Guide,

http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf0929.

Some programs in Integrative Chemistry Activities have special solicitations; see p. 10 and the Division web site, <http://www.nsf.gov/div/index.jsp?div=CHE>, for details.



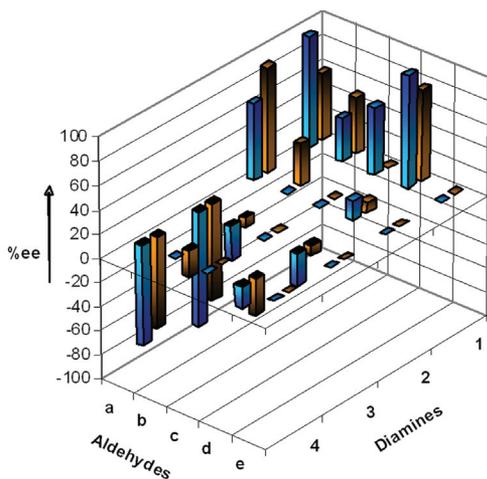
Chemical Catalysis

Program Contact: Carol Bessel
(703) 292-4945, cbessel@nsf.gov

The Chemical Catalysis Program supports fundamental experimental and theoretical research directed towards the synthesis and characterization of catalysts and pre-catalysts. This Program accepts proposals on catalytic approaches which facilitate, direct, and accelerate efficient chemical transformations and include, but are not limited to: the design and synthesis of organic, inorganic and hybrid catalytic and pre-catalytic species on the molecular, supramolecular, and nanometer scales; kinetic, mechanistic, and dynamic studies of homogeneous, heterogeneous, biomimetic and biologically-inspired catalytic reactions; characterization of chemical and biochemical catalytic reactions occurring at solid surfaces and/or interfaces; polymerization catalysis; single site catalysis; electrocatalysis (such as water splitting), photocatalysis (such as solar energy conversion); catalytic conversions of fossil fuel feedstocks, biomass conversions, CO₂ activation and other energy-related, catalytic processes; combinatorial catalysis approaches; environmentally-friendly catalytic processes; and applications of modeling, theory, and simulation to catalytic reactions.

The Chemical Catalysis Program does not support scale-up, processing, transport dynamics, long-term stability studies, and other engineering aspects of catalysis.

Biological catalysis using cellular systems (that is, systems that are not biological models or biological mimics) should be directed to other programs, e.g., Chemistry of Living Systems Program or the Division of Molecular and Cellular Biosciences (BIO/MCB) or the National Institutes of Health.



Data from high information content screening: Cobalt(III)-salen catalysts were investigated in terms of enantioselectivity (shown left), substrate specificity and relative rates of reactivity.

Credit: David B. Berkowitz, University of Nebraska.



Chemical Measurement and Imaging

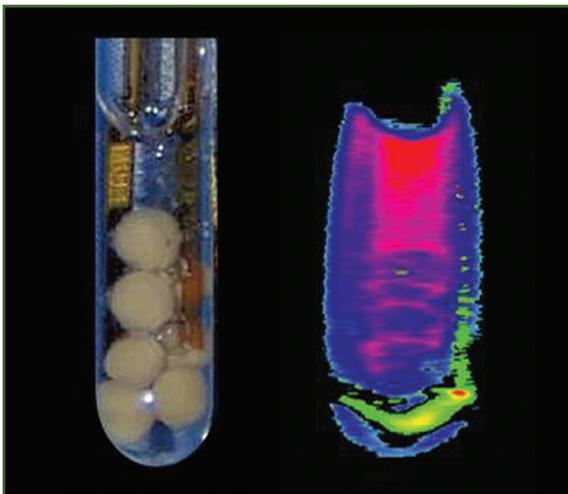
Program Contact: Kelsey Cook
(703) 292-7490, kcook@nsf.gov

The Chemical Measurement and Imaging (CMI) 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; electrochemistry; spectrometry; frequency- and time-domain spectroscopy; sensors and bioassays; and microscopy. Imaging and measurement tools probing chemical and physical properties and processes across a wide range of spatial scales - from macroscopic structures down to single molecules - are supported, as are innovations enabling the monitoring and imaging of rapid chemical and electronic processes and new approaches to data analysis and interpretation, including chemometrics. Proposals addressing established techniques must seek improved understanding and/or innovative approaches to substantially broaden applicability.

Proposals for applying established methods to applications should be directed to programs focused on the application. There are closely-related programs in other Divisions; where to submit depends on the primary focus of the proposed research.

A magnetic resonance image illustrates that the mechanical flow dispersion of pure water entering a water-filled tube packed with large beads can be directly visualized without using specialized imaging techniques or tracers.

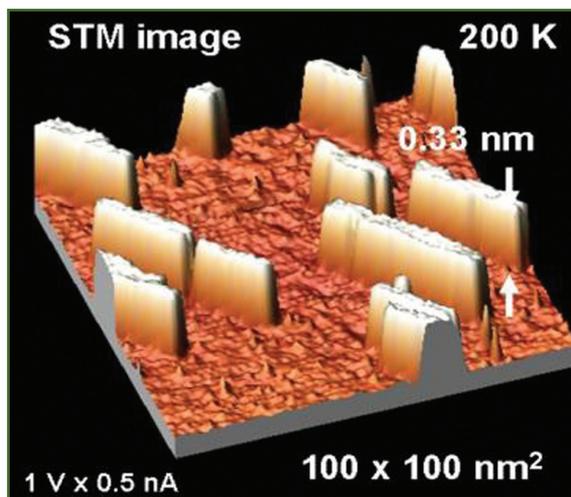
*Credit: Songi Han,
University of California at
Santa Barbara.*



Chemical Structure, Dynamics and Mechanisms

Program Contact: Colby A. Foss
(703) 292-8404, cfoss@nsf.gov

The Chemical Structure, Dynamics and Mechanisms Program supports basic, transformative experimental and theoretical research directed toward elucidating electronic and molecular structure, structure-activity relationships, dynamic interactions at the molecular level and chemical reaction mechanisms. The program is particularly interested in hypothesis-driven or exploratory research projects that address grand challenges in the field of chemistry including, for example, understanding the principles of chemical reactivity in homogeneous, heterogeneous and interfacial systems and the use of advanced computational and spectroscopic techniques to address chemical systems at the limits of temporal and spatial resolution. The program supports studies that focus on the dynamic behavior and chemical reactions of molecules and atomic and molecular clusters, in the gas, liquid, and solid phases. Specific examples include studies of the dynamics of photochemical reactions and charge transfer processes and studies aiming to understand and control light-matter interactions at the molecular level. The program also supports the use of experimental, modeling and computational techniques to probe the orientation, interactions and reaction mechanisms of molecular species on surfaces and at other interfaces.



An image of a formation of 2-atom-high bilayer islands of Ag by deposition on NiAl(110) at 200 K. The bilayer growth is guided by quantum size effects.

Credit: Patricia Thiel and Jim Evans, Iowa State University.

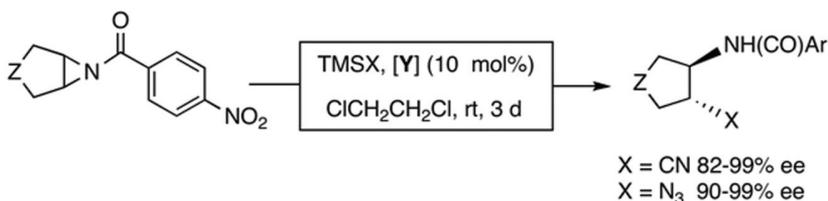


Chemical Synthesis

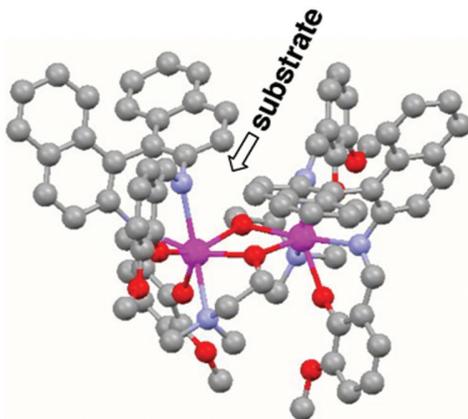
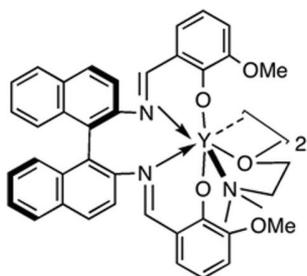
Program Contact: Tingyu Li
(703) 292-4949, tli@nsf.gov

The Chemical Synthesis Program focuses on the development of new, efficient synthetic methodologies and on the synthesis of complex molecules and molecular ensembles. Typical synthetic targets involve novel structures, structures displaying unique properties, or structures providing pathways to discover and elucidate new phenomena. Examples of supported research areas include the development of innovative reagents, catalysts for synthetic transformations, discovery of new synthetic methods, target-oriented synthesis, green synthesis, and synthesis of novel organic, organometallic, and inorganic structures. Research in this program will generate fundamental knowledge of chemical synthesis that enables the development of new avenues of basic chemical research and transformative technologies.

The Chemical Synthesis Program does not support projects whose main objective is on the property of the systems even though it may involve a large synthetic component.



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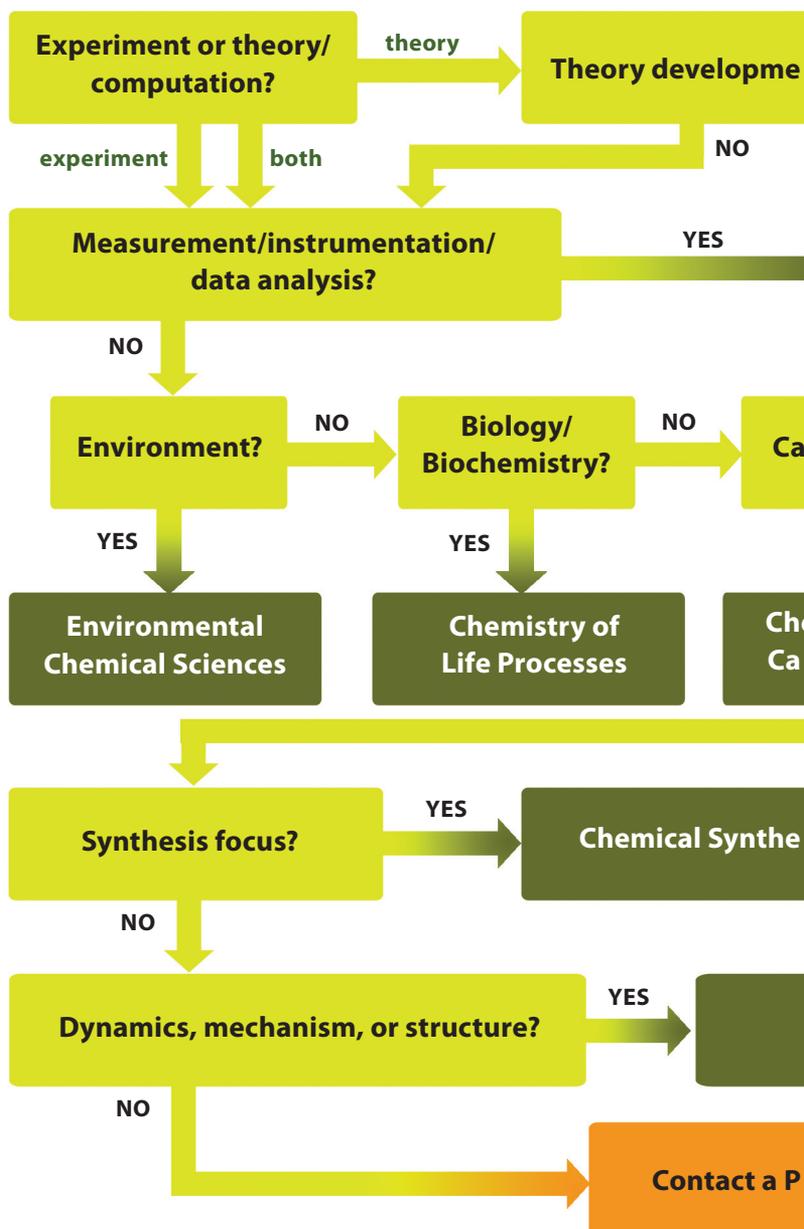


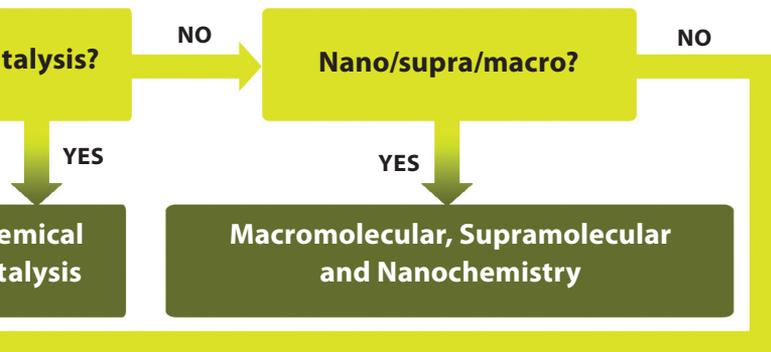
The resolving power of metals: dimeric yttrium-salen complexes, prepared from commercially available reagents, catalyze highly enantioselective ring opening of meso-aziridines.

Credit: T. V. RajanBabu and Jon Parquette, The Ohio State University.



Finding a Home for an Unsolicited Proposal

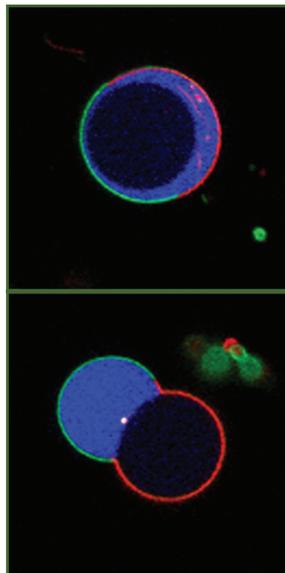




Chemistry of Life Processes

Program Contact: Wilfredo Colón
(703) 292-8171, wcolon@nsf.gov

The Chemistry of Life Processes program deals with the investigation of novel chemistry in biological systems and the advancement of basic chemical research and transformative technologies through creative applications that address important aspects of life processes. Research of interest to the program includes fundamental chemistry-centered projects at the interface with biology. The program also welcomes projects that integrate experimental and theoretical approaches, as well as inter- and multi-disciplinary research efforts at the chemistry-biology interface. Some examples include but are not limited to: synthetic methods for site-specific modifications of macromolecules; the application of advanced spectroscopic techniques to study energy transformations in biological systems; metal speciation, coordination and function; chemical (“bottom-up”) synthetic biology; chemical basis of ligand-macromolecule recognition; studies of enzyme and ribozyme catalysis that focus on the chemistry; and the design and synthesis of riboswitches and small molecules that modulate biological systems. The program also encourages research projects that exploit biological systems to advance fundamental and enabling aspects of chemistry. Proposals that are compatible with the program are those that advance the knowledge and practice of chemistry. Proposals that focus mainly on addressing a biological question are more appropriate for the Division of Molecular and Cellular Biosciences (MCB). Proposals that address biomedical problems may be more appropriate for the National Institutes of Health.



Top: Image of a model cell. The blue region is polyethyleneglycol (PEG), which is concentrated in the outer polymer solution; the green area is the portion of the membrane that contains PEG groups, which interact with the contents of the cell; and the red area is the portion of the membrane with fewer PEG groups, which interact with the contents of the cell to a lesser extent.

Bottom: After exposure to a concentrated solution of sugar, the cell converts to a budded form.

Credit: Christine Keating, Pennsylvania State University.

Environmental Chemical Sciences

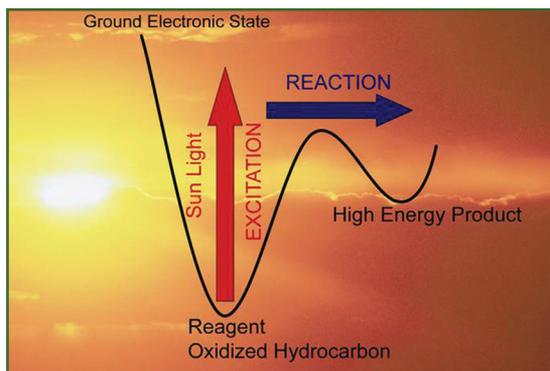
Program Contact: Zeev Rosenzweig
(703) 292-7719, zrosenzw@nsf.gov

The Environmental Chemical Sciences (ECS) Program supports basic research in chemistry that promotes the understanding of natural and anthropogenic chemical processes in our environment. Projects supported by this program enable fundamentally new avenues of basic research and transformative technologies. The program is particularly interested in studying molecular phenomena on surfaces and interfaces in order to understand the inherently complex and heterogeneous environment. Projects utilize advanced experimental, modeling and computational approaches, as well as developing new approaches. Topics include studies of environmental surfaces and interfaces under laboratory conditions; the fundamental properties of water and water solutions important in environmental processes; dissolution, composition, origin and behavior of molecular scale systems under a variety of naturally occurring environmental conditions; chemical reactivity of synthetic nanoparticles and their molecular level interactions with the environment; and application of theoretical models and computational approaches to discover and predict environmental phenomena at the molecular scale.

The ECS program supports research in basic chemical aspects of our environment. Programs in the Biological Sciences, Engineering and Geosciences Directorates as well as other funding agencies address other aspects such as field studies.

Schematic view of the sunlight-initiated generation of high energy compounds.

Credit: Veronica Vaida/Kaito Takahashi, University of Colorado at Boulder.



Integrative Chemistry Activities

Program Contact: Katharine J. Covert
(703) 292-4950, kcovert@nsf.gov

The Integrative Chemistry Activities (ICA) Program is a family of programs that supports all areas of science covered by the Division of Chemistry (CHE). Integrative Chemistry Activities programs include special projects (workshops, educational efforts, etc.) that span all of Chemistry, chemistry submissions to NSF-wide programs such as Research Experiences for Undergraduates (REU; http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf07569) and Major Research Instrumentation (MRI; http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf09502), plus the following solicitations:

- **Chemistry Research Instrumentation and Facilities**
(CRIF; http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf09546)
- **Centers for Chemical Innovation**
(CCI; http://www.nsf.gov/funding/pgm_summ.jsp?pims_id=502106&org=CHE&from=home)
- **American Competitiveness in Chemistry Fellowships**
(ACC Fellows; http://www.nsf.gov/publications/pub_summ.jsp?ods_key=nsf08541)



2008 Research Experiences for Undergraduates (REU)/Research Experiences for Teachers (RET) participants at The University of Alabama:

Back Row (l to r): Dr. John Vincent, Carl Saint-Louis, Awuri Asuru, Kim Anderson, Daniel Sweat, Craig Goodwin, Cynthia Kaeser, Deborah Harper, Jessica Hinton, and Dr. Stephen Woski.

Front Row (l to r): Brenda O'Neal, Amber Beg, Nicole Blewitt, Angelica Trumer, Felicia Briggins, CharLe Guyton, Rajini Murthy, Ashley Casey, Camille Makarem, and Jane Moore.

Credit: John B. Vincent and Stephen A. Woski, Department of Chemistry, The University of Alabama.

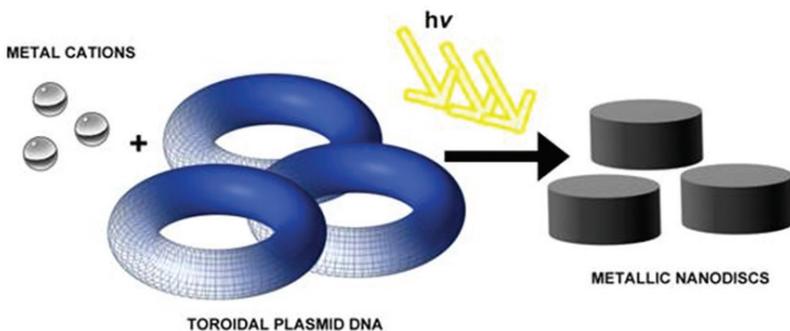


Macromolecular, Supramolecular and Nanochemistry

Program Contact: Timothy Patten
(703) 292-7196, tpatten@nsf.gov

The Macromolecular, Supramolecular and Nanochemistry (MSN) Program focuses on basic research in chemistry that addresses interactions leading to the assembly of macromolecular, supramolecular and nanoscopic species and other organized structures that show unique chemical and physical properties and reactivities. Research of interest to this program includes: the study of forces which are responsible for spatial organization in organic, inorganic or hybrid systems; novel synthesis relevant to the program topics; innovative surface functionalization chemistry; and the formation of clusters, aggregates, nanoparticles and large molecular architectures. Interactions that give rise to molecular self assembly, metal organic frameworks, template-directed syntheses, and chemically dynamic systems like molecular machines are also appropriate for this program. Investigations may utilize experimental and/or computational methods to predict and/or understand the chemical structure, properties and reactivities of these unique structures.

One objective of the MSN Program is to bridge the gap between molecular chemistry and materials science and engineering. The MSN Program works closely with NSF Divisions of Materials Research (DMR) and Civil, Mechanical and Manufacturing Innovation (CMMI) to evaluate proposals at these interfaces.



Simple DNA rings (plasmids) can be used to template formation of metallic nanodiscs.

Credit: Charles Michael Drain, Hunter College of the City University of New York.

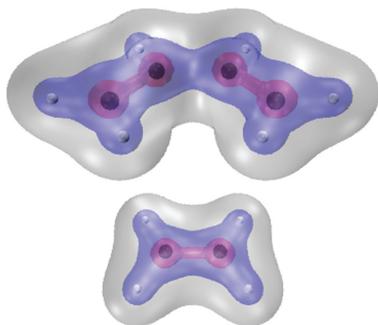


Theory, Models and Computational Methods

Program Contact: Evelyn Goldfield
(703) 292-2173, egoldfie@nsf.gov

The Theory, Models and Computational Methods program supports the discovery and development of theoretical and computational methods to address a range of chemical challenges, with emphasis on emerging areas of chemical research. Proposals that focus on established methods should involve innovative approaches that substantially broaden their applicability. Methods of interest include, but are not limited to, those addressing electronic structure, quantum reaction dynamics, statistical mechanics, molecular dynamics, and simulation techniques for molecular or supramolecular systems. Areas of application span the full range of chemical systems from small molecules to macromolecules and degrees of aggregation from single molecules or small clusters to nanoscopic and even larger systems. While application areas may involve any chemical system, including biological systems or materials, the goal of the program is to support the development of new theoretical and computational methodologies that will be broadly applicable to a range of challenging problems. We are particularly interested in fundamental areas of research that are difficult or impossible to address using current synthetic, experimental, and/or computational methodologies.

Proposals that utilize well-established theoretical and modeling approaches to solve chemical problems may be more appropriate for other divisional programs. Proposals that focus primarily on addressing biological or biomedical problems may be more appropriate for the Division of Molecular and Cellular Biosciences (MCB) or the National Institutes of Health, respectively. Proposals whose major focus is on the development of methods to improve the properties of materials should be directed to the Division of Materials Research.



Simulation of a Diels-Alder reaction via direct dynamics: a moving ethylene (C₂H₄) molecule (lower part) encounters a stationary 1,3-butadiene (C₄H₆) molecule (upper part) to form a cyclohexene (C₆H₁₀) molecule. The clouds represent the electronic charge densities of the molecules.

*Credit: Jorge A. Morales,
Texas Tech University.*

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Web site: <http://www.nsf.gov/div/index.jsp?org=CHE>

Division Director, Luis A. Echegoyen
(703) 292-4960, lechevoy@nsf.gov

Executive Officer, Janice M. Hicks
(703) 292-4956, jhicks@nsf.gov

Division of Chemistry Programs

Each program will be staffed by multiple Program Directors with complementary expertise.
Inquiries may be directed to the program contacts listed below:

Chemical Catalysis

Contact: Carol Bessel
(703) 292-4945, cbessel@nsf.gov

Environmental Chemical Sciences

Contact: Zeev Rosenzweig
(703) 292-7719, zrosenzw@nsf.gov

Chemical Measurement and Imaging

Contact: Kelsey D. Cook
(703) 292-7490, kcook@nsf.gov

Integrative Chemistry Activities
Program Contact: Katharine J. Covert
(703) 292-4950, kcovert@nsf.gov

Chemical Structure, Dynamics and Mechanisms

Contact: Colby A. Foss
(703) 292-8404, cfoss@nsf.gov

Macromolecular, Supramolecular and Nanochemistry

Contact: Timothy Patten
(703) 292-7196, tpatten@nsf.gov

Chemical Synthesis

Contact: Tingyu Li
(703) 292-4949, tli@nsf.gov

Theory, Models and Computational Methods

Contact: Evelyn Goldfield
(703) 292-2173, egoldfie@nsf.gov

Chemistry of Life Processes

Contact: Wilfredo Colón
(703) 292-8171, wcolon@nsf.gov