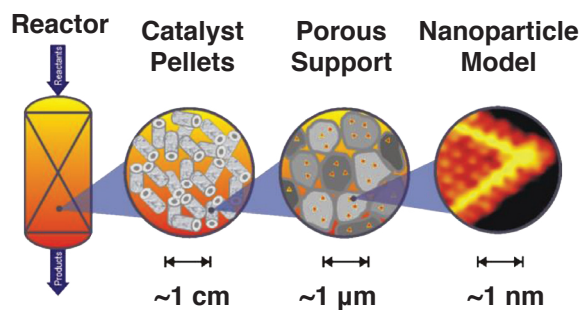
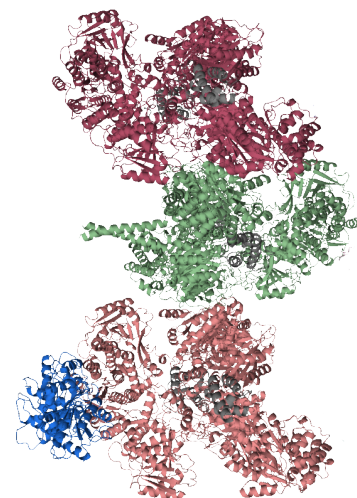
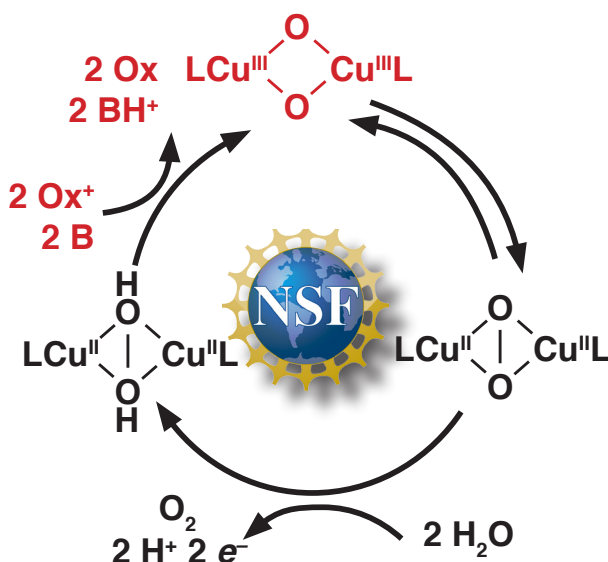
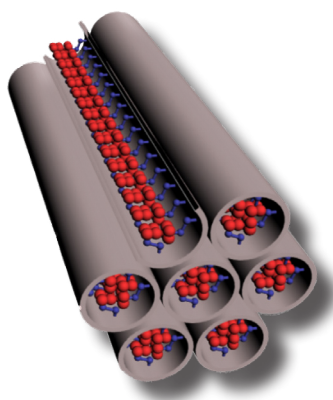
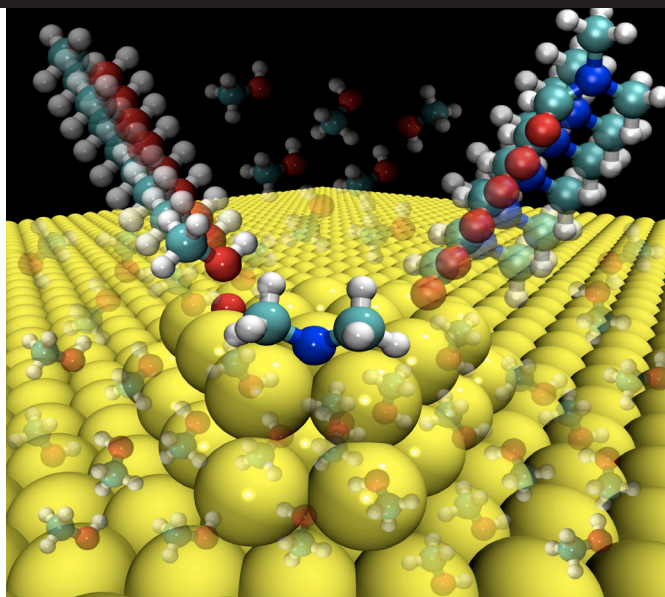


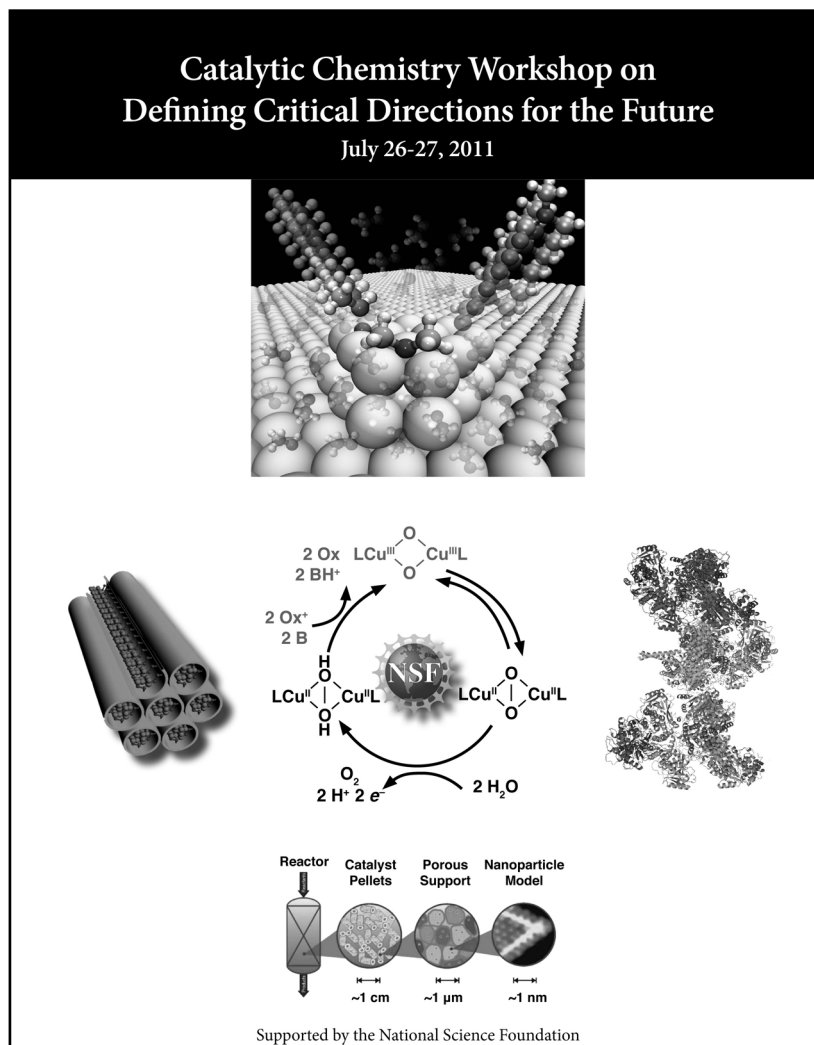
Catalytic Chemistry Workshop on Defining Critical Directions for the Future

July 26-27, 2011



Supported by the National Science Foundation

Catalysts on the cover: (from top clockwise): Schematic mechanism for dimethylformamide synthesis from methanol coupling with dimethyl amine via a $(\text{CH}_3)_2\text{N}$ intermediate on Au activated by oxygen courtesy of Bingjun Xu; assembly line biocatalyst used in transforming simple building blocks into complex organic molecules; courtesy of Shiven Kapur, Alice Chen, David Cane, and Chaitan Khosla [1]; illustration of the structure, length scales, and complexity involved in modern catalysts courtesy of inano.au.dk; and heterogeneous acid catalysts incorporated into mesoporous silica for carbohydrate dehydration courtesy of A. Crisci and S.L. Scott [2] surround a catalytic cycle for electrolytic water oxidation by copper-bipyridine-hydroxo complexes recently proposed by S. Barnett, K. Goldberg, and J. Mayer [3].



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Executive Summary

Catalytic chemistry plays a vital role in the world economy since it is a key technology for chemical and materials synthesis, fuel production, power generation, and conversion and environmental remediation. Catalysis research is a major driver for the development of sustainable processes for fuel production and for synthesis of materials and chemicals [1-3]. Among the critical technologies that rely on catalysis are efficient synthesis of chemicals and pharmaceuticals, petroleum biomass conversion to fuels and platform chemicals, and production of materials for solar energy utilization, storage, and energy-efficient consumer and building products. A fundamental understanding of all areas of catalysis—homogeneous, heterogeneous, biological, photochemical, and electrochemical—is needed to develop more sustainable processes.

The new alignment of programs within the Chemistry Division (CHE) at the National Science Foundation (NSF) recognizes the central role of catalysis by establishing a new program to keep our nation's effort at the forefront of catalysis research. A workshop on chemical catalysis was proposed to NSF CHE. The workshop was held in conjunction with the American Chemical Society (ACS) meeting held in Denver, Colorado in August 2011 to discuss current research as well as to identify future challenges and opportunities in this field that would benefit the catalysis community.

Critical Directions for Catalysis

Through presentations, extended discussions, and working group meetings, the workshop attendees developed the following critical directions to the advancement of the nation's catalysis effort:

1. Robust funding of catalysis is crucial to maintaining the nation's competitiveness. The workshop participants strongly endorsed catalysis-funding reflect the full breadth of research areas represented at the workshop and focus on support of fundamental research.
2. Catalysis funding should support graduate student and postdoctoral fellowships that will allow researchers to gain experience across the areas of catalysis and provide supplemental funding to grants in the program to promote collaboration across the different areas of the program.
3. An annual Catalysis Workshop should be held in conjunction with one of the American Chemical Society (ACS) national meetings to further build stronger ties in catalysis across the chemistry community.
4. The workshop attendees urged the funding by federal agencies of 1-3 Regional Instrumentation Centers (\$20M capital investment and \$5M/yr for operational support per Center) to provide the essential state-of-the-art instrumentation needed for the nation's catalysis research. These Instrumentation Centers should incorporate data storage and mining to enhance capability for directed and rapid design of catalytic materials and processes [4].
5. Given that catalysis plays such a vital role in many key processes, the workshop participants suggested that catalysis program officers continue to work synergistically, and with across larger federal programs, such as the Science, Engineering and Education for Sustainability (SEES) program at NSF, to garner additional support for activities including postdoctoral fellowships or joint workshops.

With strong support for basic research in catalysis, U.S. leadership in this core field will continue to advance. The investment in students associated with this effort is also essential to the development of the next generation of well-trained chemists in this area who represent the future scientific capital for the country. These critical directions focus on ensuring U.S. leadership in this intellectually exciting field that is technologically and economically vital to the nation.

Introduction

Catalytic chemistry is central to the world economy since it is a key technology for chemical and materials synthesis, fuel production, power generation, and conversion and environmental remediation. The critical importance of catalysis is illustrated by the fact that six recent Nobel Prizes in Chemistry [see **Nobel Prizes in Catalysis in the 21st Century**] have recognized contributions to catalytic science [5]. The new alignment of programs within the Chemistry Division at NSF has also recognized the central nature of catalysis and of the pivotal role of chemical sciences in catalysis by establishing a new program that has the potential to revolutionize research in this field.

A workshop was proposed to bring together a group of leaders and emerging leaders in catalysis research [Figure 1] to exchange ideas, identify future challenges and opportunities in this broad-reaching field and to identify critical directions that would benefit the catalysis community.

The importance of catalysis stems from the fact that essentially all chemical and materials syntheses rely on a catalytic process in at least one step along the way [see **Catalytic Assembly Line**]. The major impact of catalysis on our economy [6] and on the field of chemistry is described in several major reports [7-8]. Catalysts are materials—solids, nanoparticles, enzymes, molecules, and porous frameworks, for example—that are neither consumed nor produced in a process, but that increase the rate of a chemical transformation by providing low energy pathways. Catalysts function by introducing one or more elementary chemical steps that are more facile than the steps required in their absence. An ideal catalyst also directs the reaction to a single desired product, so as to minimize waste and avoid the production of potentially harmful by-products.

Catalytic processes enhance efficiency by decreasing the temperature for specific chemical syntheses and by increasing the selectivity—the preference for the desirable product over all others. The production of carbon emissions from chemical synthesis provides an example of the enormous impact of chemical production on our environment and on the world economy [see **Impact of Chemical Productions on the Environment**]. Because catalysis plays such an important role in chemical and fuel production, advancement in catalytic chemistry is an essential element for improving energy efficiency and minimizing environmental impact.

Catalytic processes are central to our economy and quality of life. Catalysts are an enabling technology for the production of fertilizers so that food production maintains pace with population growth. Processing of fossil fuels for energy production and transportation also relies heavily on catalysts in order to produce high-value and clean fuels. Syntheses of most chemicals and of polymeric materials, used widely in our society, also depend on catalysts. Even though these are well-established processes, there is a need for enhancing these technologies because of increasing demand for diminishing resources.

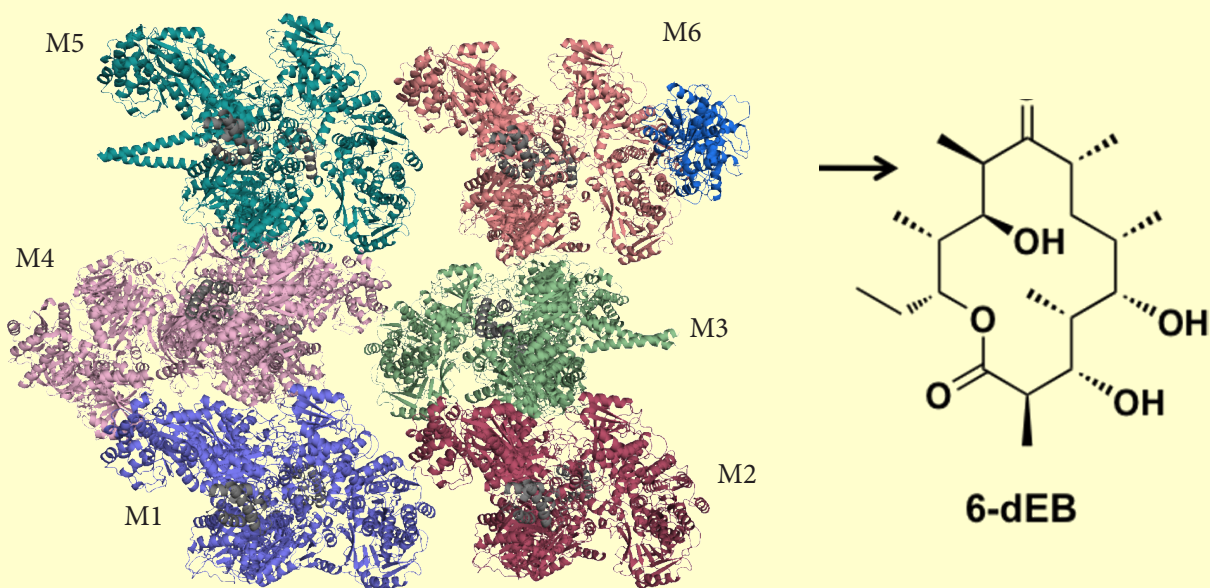
Nobel Prizes in Catalysis in the 21st Century



The critical importance of catalysis is illustrated by the fact that six recent Nobel Prizes in Chemistry have recognized contributions to catalytic science.

- **2001** to *William S. Knowles* and *Ryoji Noyori* “for their work on chirally catalyzed hydrogenation reactions” and to *K. Barry Sharpless* “for his work on chirally catalyzed oxidation reactions”
- **2005** to *Yves Chauvin*, *Robert H. Grubbs*, and *Richard R. Schrock* “for the development of the metathesis method in organic synthesis”
- **2006** to *Roger D. Kornberg* “for his studies of the molecular basis of eukaryotic transcription”
- **2007** to *Gerhard Ertl* “for his studies of chemical processes on solid surfaces”
- **2009** to *Venkatraman Ramakrishnan*, *Thomas A. Stietz*, and *Ada E. Yonath* “for studies of the structure and function of the ribosome”
- **2010** to *Richard F. Heck*, *Ei-ichi Negishi*, and *Akira Suzuki* “for palladium-catalyzed cross couplings in organic synthesis”

Catalytic Assembly Line



Using assembly line catalysts is a new theme emerging in the field of biocatalysis. It offers unique opportunities for transforming simple building blocks into complex organic molecules in an atom-economical manner. As illustrated above, the 6-deoxyerythronolide B synthase (MW ~ 2 MDa) converts one equivalent of propionyl-CoA and six equivalents of (2S)-methylmalonyl-CoA into a macrocyclic product using NADPH as a hydride source. A fundamental challenge to the understanding of such assembly lines is the ability to explain how the biosynthetic intermediate is translocated in a unidirectional manner over distances that can often exceed 100 nm. To this end, atomistic structural models have recently been developed of the 6-deoxyerythronolide B synthase which demonstrate that protein-protein interactions play a crucial role in substrate channeling across the assembly line. (Taken with permission from [1] S. Kapur *et al.*, *PNAS* **107**(51): 22066-22071, 2010 and C. Khosla *et al.*, *Annu. Rev. Biochem* **76**: 195-221, 2007)

Catalysis also has a major impact on the environmental consequences of transportation and synthesis. The best-known example is the development of “catalytic converters” in automobiles that have dramatically reduced the emissions of NO_x and uncombusted hydrocarbons from our vehicles; thus, leading to major improvements in air quality over the past few decades. Nevertheless, there is still need for improvement in these processes given the growth in automobiles worldwide.

Looking to the future, catalysis also has a central role to play in alternative energy production and conversion [6]. Processing of biomass into fuel, for example, will rely heavily on catalytic processes. Photocatalysis has the potential to produce fuels, *e.g.*, via light-driven water splitting. Electrocatalysis is key for fuel cell technologies and electrical energy storage in, for example, batteries and supercapacitors. These emerging areas require the creative

design of materials, especially at the nanoscale, and an understanding of key processes.

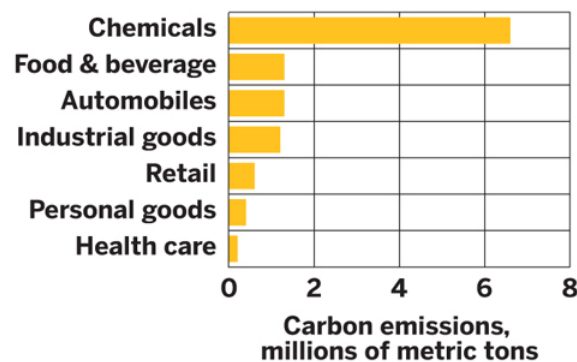
All of these areas in which catalytic chemistry plays, depend on the discovery and development of new materials and molecules for these processes and on a fundamental understanding of how specific catalysts function, in order to design new processes. Thus, future research in catalysis must involve (1) synthesis of new catalysts—both homogeneous and heterogeneous; (2) theoretical descriptions of their properties; (3) establishment of the fundamental underpinnings for the function of effective catalysts; and, (4) identification and development of new enabling technologies and resources.

Because catalysis is a cross-cutting discipline that spans numerous fields—including inorganic chemistry, solid state chemistry, synthetic organic chemistry, condensed matter physics, biochemistry,

Impact of Chemical Productions on the Environment

CARBON FOOTPRINT

Average S&P 500 chemical company emits 6.6 million metric tons of carbon



NOTE: Data represent 2007 average emissions for companies in each sector of the S&P 500 presented.
SOURCES: NSF International, Trucost

Chart showing the significant impact of chemical production on carbon emissions. (Used by permission from C&EN, August 31, 2009, 87(35), 10. by Marc S. Reisch).

electrochemistry, and nanoscience—defining these directions require participation by chemists and other scientists in a range of disciplines. The workshop was designed to engage participants from a broad range of areas:

(1) heterogeneous catalysis and surface chemistry, (2) homogeneous catalysis and organic synthesis, (3) biological and bio-inspired catalysis, (4) photocatalysis, and (5) electrocatalysis.

The workshop drew together a diverse group of established and emerging leaders in catalysis [Figure 2] in order to highlight the challenges and the future directions in the field [see Appendix I]. By engaging a diverse group of catalysis research, the workshop looked to define areas to advance the field as a whole, identify critical needs to advancing the field, and develop strategies for training the next generation of chemists in this field.

Goals and Format for the Workshop

The goals of the workshop were to establish a vision

for catalysis research in the NSF CAT program for the future. The workshop was designed to provide a background on the current cutting-edge research and to identify areas with high priority for funding in the future. The specific goals of the workshop were:

1. To define key areas of study relevant to sustainable production and conversion of chemicals, energy and pharmaceuticals for the NSF CHE Catalysis program.
2. To identify key resources, including instrumentation and computational capabilities, required for impact on the high priority scientific areas identified.
3. To identify funding mechanisms, such as individual investigator, small group, or center funding, that will enhance and accelerate progress in catalysis research.

Within this framework, the workshop participants were asked to delineate the distinctive characteristics of the NSF CAT program and to specifically differentiate it from corresponding programs funded by the Department of Energy (DOE) programs in Basic Energy Sciences (BES), and the Chemical and Biological Engineering and Technology (CBET) program at NSF. The workshop was organized to engage participants from a broad range of areas: (1) heterogeneous catalysis and surface chemistry, (2) homogeneous catalysis and organic synthesis, (3) biocatalysis, (4) photocatalysis, and (5) electrocatalysis. The

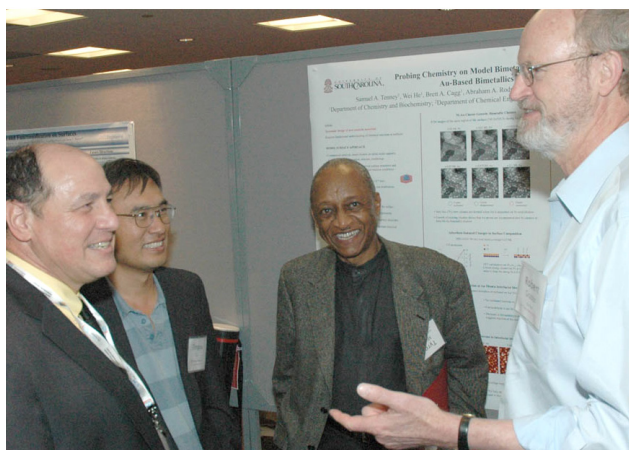


Figure 1. Drs. Matthew S. Platz, Tingyu Li, and Tyrone Mitchell, from the National Science Foundation, talking with Professor Robert Grubbs, California Institute of Technology and Nobel Laureate in Chemistry, during the poster session.



Figure 2. Participants in the Catalytic Chemistry Workshop.

aim was to involve a diverse group of participants, with wide intellectual, geographic, gender, and ethnic diversity at a variety of different career stages. This approach was designed to provide the most valuable outcome to serve the catalysis community.

The format of the workshop was designed to elicit a broad range of input from the participants and their respective fields [Appendices II and III]. The workshop consisted of three stages: (1) presentation of research directions, challenges, and opportunities by participants in the form of poster and oral presentations, supplemented by an overview presentation of co-chair, Cynthia Friend [Figure 3]; (2) discussion and distillation of the material in the form of smaller “break-out” groups; and (3) report back from the break-out groups and general discussion leading to an outline for the workshop report.

Support for Catalysis from Federal Agencies

There are several Federal programs that currently fund catalysis research.

The *National Science Foundation's Chemical Catalysis Program* supports experimental and theoretical research directed towards the fundamental understanding of the chemistry of catalytic processes at the molecular level. The NSF CAT Program accepts proposals on catalytic approaches, which facilitate, direct, and accelerate efficient chemical transformations. This includes the design and synthesis of catalytic and pre-catalytic species on the molecular, supramolecular, and nanometer scales; and studies of the dynamics of homogeneous and heterogeneous catalytic processes. Processes of research interest may vary with demands and progress in certain areas. The overarching goal is to control the chemistry (*e.g.*, polymerization or asymmetric catalysis) through the design of the catalyst sites (*i.e.*, uniformity or substrate-specificity) including biologically-inspired catalysis. Applications of modeling,

theory, and simulation to catalytic processes are also relevant.

Research submissions that advance chemical catalysis and address national needs for sustainability are of particular interest. These include fundamental studies of energy-related catalytic processes, CO₂ conversion, electrocatalysis (such as in water splitting and fuel cells), photocatalysis (such as in solar energy conversion), catalytic conversions of fossil fuels and biomass, and environmentally-friendly chemical processes. The Program does not support applied catalysis research that focuses on scale-up, processing, transport dynamics, long-term stability and other engineering aspects of catalysis. The Program also does not support biocatalysis research with purely biological enzymes and cellular systems.

The *NSF's Chemical and Biological Engineering and Technology (CBET) Program* encompasses a blend of fundamental and innovative applied research drivers. All programs are hypothesis-driven, and the experimental programs aimed at resolving the issues frequently combine a variety of approaches. Chemical engineering and chemistry are intertwined. Proposals, which receive funding in this Program may include any number of the following broad scopes:

- Catalyst Synthesis, Characterization, Behavior and Performance
- Kinetics and Mechanisms of Key Catalytic Reactions
- Catalysis at Surfaces or in Reactor Process Streams
- Synthesis and Fabrication of Component Materials and Catalyst Composites
- Modeling and Fundamental Studies of a Catalyst or Catalytic Process
- Catalysts and Studies for Renewable Energy Systems.

These approaches apply equally to classical inorganic or carbon catalysts as well as to enzymatic or

biocatalysts. Specialized materials synthesis procedures may be necessary to provide active catalysts in any of the studies. Application-driven studies, such as Biomass Conversion Catalysis, Electrocatalysis, and Photocatalysis, involving energy interconversion devices or systems employing catalysts are highly desired

Most studies will focus on the catalysis of one or more chemical reactions with products including molecules used for fuels, energy sources, feedstocks, fine chemicals, bulk chemicals, and specialized materials. While proposals will be accepted in any of the above areas, national needs suggest heightened interest be given to proposals relating to processes and catalysts for conversions of biomass to fuels and chemicals, for development of renewable energy sources and for transition to green or

environmentally benign products and processes. Submissions investigating unique nanoparticle or biomimetic catalysis are welcome.

The *Department of Energy's Division of Chemical Sciences, Geosciences, & Biosciences (CSGB)* supports research that develops the fundamental scientific principles enabling rational catalyst design and chemical transformation control. Research includes the identification of the elementary steps of catalytic reaction mechanisms and their kinetics; construction of catalytic sites at the atomic level; synthesis of ligands, metal clusters, and bio-inspired reaction centers designed to tune molecular-level catalytic activity and selectivity; the study of structure-reactivity relationships of inorganic, organic, or hybrid catalytic materials in solution or supported on solids; the dynamics of catalyst structure relevant to



Figure 3. (Clockwise from top left) *Professor Cynthia Friend introducing Dr. Matthew S. Platz, Director of the NSF Chemistry Division for his keynote address; Professor Frank J. DiSalvo, Cornell University, giving a keynote address on sustainability; Professor Kristala Prather, Massachusetts Institute of Technology, speaking in the bio-inspired catalysis session; and Professor Anne McNeil, University of Michigan, discusses her poster with Professor Stefan Bernhard, Carnegie Mellon University.*

catalyst stability; the experimental determination of potential energy landscapes for catalytic reactions; the development of novel spectroscopic techniques and structural probes for *in situ* characterization of catalytic processes; and the development of theory, modeling, and simulation of catalytic pathways. Capital equipment funding is provided for items such as ultrahigh vacuum equipment with various probes of interfacial structure, spectroscopic analytical instrumentation, and specialized cells for *in situ* synchrotron-based experiments, and computational resources.

Catalytic transformations impact an enormous range of DOE mission areas. Particular emphasis is placed on catalysis relevant to the conversion and use of fossil fuels, renewable energy resources, and the creation of advanced chemicals. Catalysts are vital in the conversion of crude petroleum and biomass into clean burning fuels and materials. They control the electrocatalytic conversion of fuels into energy in fuel cells and batteries and play important roles in the photocatalytic conversion of energy into chemicals and materials. Catalysts are crucial to creating new, energy-efficient routes for the production of basic chemical feedstocks and value-added chemicals. Environmental applications of catalytic science include minimizing unwanted products and transforming toxic chemicals into benign ones, such as the transformation of chlorofluorocarbons into environmentally acceptable refrigerants.

Challenges and Opportunities in Catalysis

During the afternoon of the workshop, the attendees participated in working subgroups [Figure 4]. This section reports on key challenges and opportunities that were identified for the heterogeneous, homogeneous, bio-inspired, photo and electrocatalysis areas as well as those that cut across these areas. Succeeding sections report on the conclusions and critical directions from a consensus of the subgroups and workshop participants, as a whole.

Heterogeneous Catalysis and Surface Chemistry

Heterogeneous catalysis has been the cornerstone of the chemical industry for many years, but there are still a number of long-standing challenges in the field. Fundamental understanding of molecular transformations on surfaces is critical for a number of problems related to sustainability, including conversion of biomass to fuels and chemicals, and the production of commodity chemicals from re-

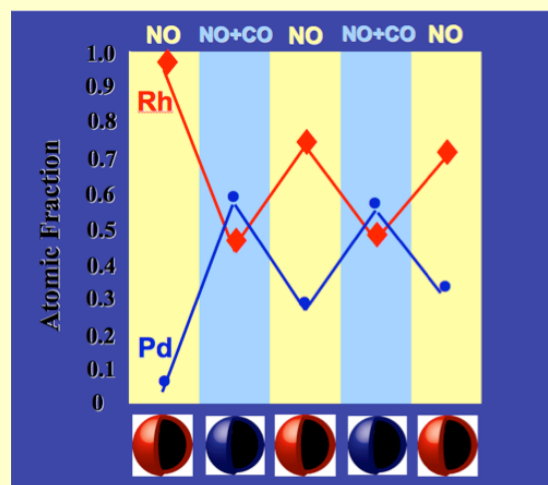
newable feedstocks.

Currently, the main challenges for heterogeneous catalysis include:

- The design of selective active sites and assemblies of active sites with molecular-level precision in order to leverage the cooperativity of these sites.
- Developing techniques to investigate the surfaces of catalytic materials which are sensitive to both organic and inorganic compounds as well as able to chemically and structurally address them.
- Understanding the principles for the design of catalyst materials that are resilient, self-healing and stable under reaction environments such as oxidizing/reducing conditions, and varying pH and temperature conditions in liquid media.

One of the keys to guiding the development of new heterogeneous catalysts is the ability to study the dynamic nature of surfaces under reaction conditions. From the experimental standpoint, the development of *in situ* analysis techniques capable of investigating the composition, structure and morphology of

Tuning Catalyst Surface Composition



The surface composition of $\text{Rh}_{0.5}\text{Pd}_{0.5}$ nanoparticles depends on reaction conditions. Oxidizing conditions—with NO present—lead to enrichment of Rh at the surface. Reducing conditions—when CO is added—have the opposite effect ([9] Tao, F. *et al.*, “Reaction-driven Restructuring of Rh-Pd and Pt-Pd Core-shell Nanoparticles,” *Science* 322: 932, 2008). These experiments are relevant to conditions in automotive exhaust catalysis.

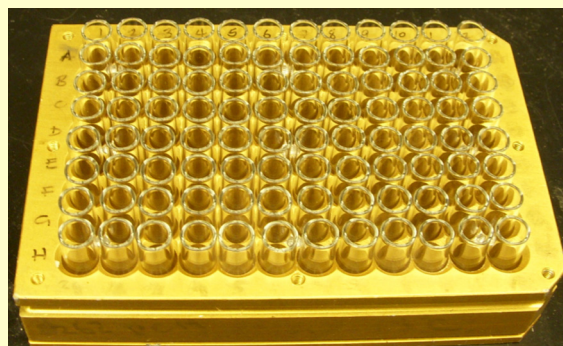
catalysts under operating conditions is a crucial advancement. For example, the sidebar (see **Tuning Catalyst Surface Composition**) shows changes in the surface composition of bimetallic Pd-Rh particles as the catalyst is exposed to gaseous reactants under operating conditions [9]. From the theoretical standpoint, the ability to predict the structures of complex materials under reaction conditions is facilitated by the continued development of multiscale modeling, improvements in the accuracy of density functional theory calculations, and advancements in the ability to handle large and complex data sets

Homogeneous Catalysis and Organic Synthesis

Homogeneous catalysis remains a vital component of chemistry research with impacts in areas as diverse as pharmaceutical chemistry, materials synthesis and target-oriented synthesis. Across all these platforms, key challenges remain in areas that are best addressed by fundamental studies enabled by the NSF, including:

- *The problem of selectivity.* In many situations, rather than reactivity, selectivity—the activation and transformation of one functional group among many—is the key challenge. A complementary and perhaps greater challenge is the selective activation of a less-reactive functional group in the presence of a more reactive one.
- *The problem of order.* Controlling the sequence of elementary reactions is another challenge. This has broad implications, from sustainable routes to controlled polymers to the cooperative action of multiple catalysts. Controlled polymerization lead to programmed materials. Multiple catalysts allow the user to intercept unstable intermediates *en route* to functionalized value-added products.
- *The problem of sustainability.* The use of earth-abundant element-derived catalysts is a desirable goal but ultimately more important to sustainability is the use of rugged, long-lived catalysts, even if they do not contain earth-abundant elements. Activation and use of renewable feedstocks is a desirable goal.
- *The problem of resources.* Research has always benefited by breakthroughs in technology. Catalysis research stands to gain immensely from various resource-intensive technology improvements. High-throughput experimentation platforms (see **High-Throughput Systems**) have been introduced that lead to reduced expense and accelerated discovery [10-11] but require in-

High Throughput Systems



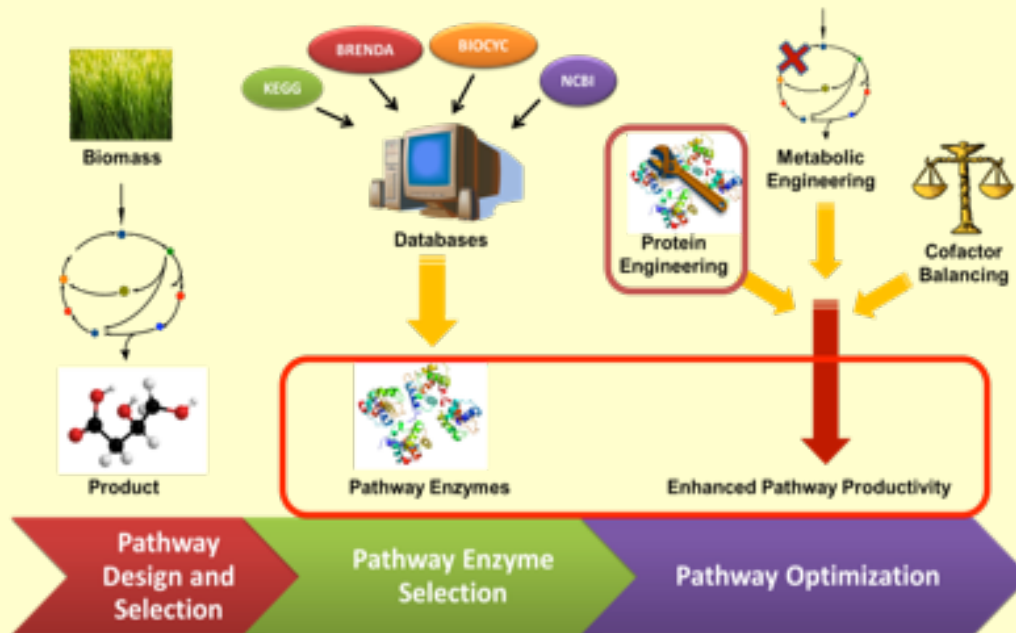
High throughput platforms (*top*) can run through 100x the number of bench reactions (*bottom*) and require smaller volumes of reagents. These systems also provide the benefit of faster turn around for more rapid reaction design.

frastructure investment as well as staff support. Access to experimentalists to computational facilities and staff would also be useful in advancing homogeneous catalysis research.

Bioinspired Catalysis

Biological synthesis is being increasingly pursued as an alternative to traditional organic synthesis for a number of products, including fuels and chemicals [12-13]. Metabolic engineering comprises a set of enabling tools and methodologies that will facilitate the emergence of these products [14-16]. The

Designing New Pathways for Biological Synthesis



Development of novel pathways for biological synthesis begins with the design and selection of a proposed route. Specific enzymes must then be selected to establish proof-of-concept for synthesis, followed by the use of a variety of tools to optimize the pathway. The boxed area is one in which fundamental research in catalysis can greatly contribute to the development of bio-based production systems. Both initial selection of enzymes and improvement of pathway productivity, especially through protein engineering, require advances in biocatalysis. (Figure adapted from [12] Dhamankar and Prather, 2011, *Curr. Opin. Struct. Biol.* **21**:488)

discipline first focused on improvement of natural producers, through the development and application of tools for rational, directed manipulation of microbial systems to increase metabolic flux. More recently, many efforts in the field involve the transference of naturally-occurring pathways from their natural hosts to heterologous ones. Reconstitution of pathways in this manner is typically desired to access more tractable hosts with a greater range of genetic tools and techniques available. However, the true emergence of a “biomass-based” economy will require not only the exploitation of naturally-occurring pathways for natural products, but also the design and construction of novel pathways for non-natural products

Key to this ability is the identification of appropriate enzymatic catalysts to comprise the microbial chemical factory (see **Designing New Pathways for Biological Synthesis**). Ideally, the choice of enzymes to mediate biotransformation of chemical substrates would be largely based on consideration of the re-

quired functional group conversion without being limited by prior evidence of transformation of the full structure. In reality, however, the ability to engineer proteins to accept novel substrates is not sufficiently advanced to adopt such an approach as a routine matter. Additionally, production of new products will require new enzymes to be identified and characterized from a broad variety of biological systems. Fundamental research in catalysis is not only a contributing factor but also a critical element in bringing these new products to market. Some challenges and opportunities in this arena are:

- *Development of improved computational methods for protein engineering.* Increasing the activity and changing the substrate range of enzymes is a critical step for novel pathways. Methods such as directed evolution can affect these properties but generally require large libraries to be screened. Better computational methods to predict sequence modifications that will lead to improved catalytic activities will greatly facilitate pathway

design, especially as high-throughput screens for many products and intermediates of interest are not readily available.

- *Understanding sequence-function relationships for catalytic specificity.* The trajectory for protein engineering is a function of the starting point. More precisely, the probability of successfully modifying the catalytic properties increases as the distance between the starting and target points decreases. Better understanding of the relationship between naturally-occurring sequences and their catalytic properties and specificity should lead to the ability to better identify the most appropriate starting points for protein engineering exercises.
- *Understanding and eliminating context dependence of catalytic activity.* Increased development of biological pathways requires increased access to enzymatic activities found in nature, either as first identified or modified as described above. Harnessing the full complement of biological catalysis requires an understanding of the context of biological activity, that is, understanding each of the factors that contribute to catalytic activity in the natural host, including accessory proteins or other co-factors as well as post-translational modifications. Importantly, this understanding should lead to an ability to minimize the number of interactions in order to facilitate transference of activities to new hosts.

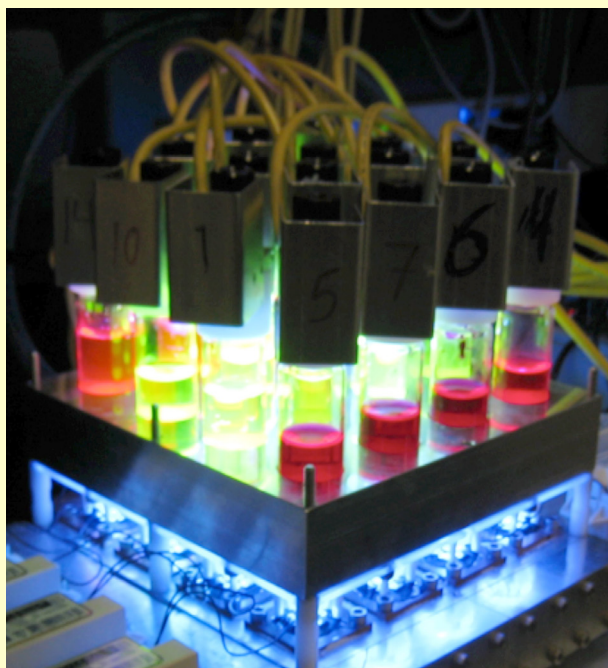
Photocatalysis and Electrocatalysis

Work in the area of photocatalysis and photo-voltaically-driven electrocatalysis is essential for the development of sustainable chemical processes. However, economic pressure has constantly driven the optimization of large-scale chemical processes (e.g., Haber-Bosch, chloralkali, water gas shift reactions) and a switch to a photochemical methodology seems less likely. In contrast, the development of novel, carbon-neutral energy cycles will have the most dramatic impact and should therefore be the target of a main thrust in area of photo- and electrocatalysis. The cleavage of water to H₂ and O₂ is an attractive concept and the research efforts directed at photo-driven water reduction and oxidation are justifiable, but it is desirable that the NSF pursues a more diversified research portfolio. Other appealing catalytic reactions such the controlled oxidation and reduction of carbohydrates, CO₂-to-fuel reduction processes, and metal oxide photolysis is a clear path to follow. The

conversion of waste streams to fuel and the chemical conversion of plant material to molecularly uniform energy carriers and commodity chemicals are also currently underdeveloped research areas. Driving such complex chemical reactions with electrons and/or photons necessitates unprecedented control of chemical reactivity and new tools have to be developed for this purpose.

- Efficient and robust catalysts for these thrusts have to be developed. A hedging approach of molecular, colloidal, and electrode-supported catalysts will ensure that photons or electrons can drive the targeted reaction. The mechanism has to be fully understood in order to improve the robustness/reactivity and allow the judicious tuning of a catalysts electrochemical and photochemical properties. The complexity of these processes dictates the development of highly parallel reactor systems for the exploration of vast parameter spaces (see **Rapid Screening of Photocatalysts**).
- Light/matter interactions are critical for photo-

Rapid Screening of Photocatalysis



Parallel photoreactor for the study of water photolysis reactions. The intricate nature of the catalytic cycles involved in such reactions necessitates the development of high-throughput screening tools.

catalytic and photo-electrochemical approaches. While simple photo-induced electron transfer processes involving molecular chromophores and semiconductors are well understood, strategies to join catalysts with a light-absorbing unit are considerably less studied. In order to prevent back-reactions, methods ensuring a photon-driven, unidirectional flow of charge through catalytic cycles need to be developed.

- The judicious design of electrodes for intricate electrocatalytic reactions is a challenge that extends far beyond the realm of traditional electrochemical approaches. Complex reactions, e.g., the formation of carbon-carbon bonds during the electrochemical reduction of CO₂, will require a complete control over the involved electron and proton transfer processes as well as enzyme-like electrode surfaces for spatially arranging the reagents.
- New analytical tools are needed for the elucidation of solution and interface-based catalytic processes. Chemists are ill-equipped for collecting structural information on reactive, low-concentration intermediates that form during catalytic processes. The nature of photo and electrocatalytic processes intrinsically leads to the formation of open-shell species that are notoriously difficult to characterize so the development of parallel analytical technology is desirable.
- Computational methods for efficient modeling and prediction of catalytic reactivity and processes are needed for understanding and accurately predicting complicated catalytic cycles. This challenge is especially apparent when reactions that proceed in protic solvent environments are investigated. A valuable objective of these efforts to link calculated intermediate structures and their reaction kinetics to experimental responses observed with electronic absorption, EPR, and electrochemical techniques.

Cross-cutting Activities and Computational Catalysis

Several of the working subgroups identified the establishment of shared facilities, possibly in regional centers, along with the essential support staff to train the next generation of catalysis researchers. Another important cross-cutting theme was the need to fund theory and computational methods that support experimental efforts in these areas. Indeed, methods such as Density Functional Theory (DFT) have

become an essential tool in relating atomic-level mechanisms to catalyst reactivity.

DFT is currently used to interpret a range of experimental *in situ* probes in ultrahigh vacuum and high-pressure surface science studies along with *in operando* studies under reaction conditions. Increasingly DFT has also been used to design novel catalysts through computational screening using identified key descriptors that predict catalyst performance. Despite the great successes of DFT, there are limitations due to the computational cost of these calculations. One is the length and time scales that can be directly probed. The current limits of *ab initio* molecular simulations are on the nanosecond scale and recent DFT calculations have been performed on ~ 4 nm metal nanoparticles. While this length and time scale is sufficient to probe local reconstructions and nanoparticle size effects, it is not possible to follow large-scale changes to the catalyst surface under reaction conditions.

The sidebar on **Catalysis by Design** shows STM images from Varga and co-workers [17] of the 2D oxide phases that form on Pd(111). With the help of DFT they were able to resolve the atomic-level structure of the 2D phases and they reported a Pd₅O₄ phase that has no direct relationship to bulk PdO. The evolution of such phases could not be predicted *a priori* with DFT, but the details of the structure of the oxide phases that form in between the transition from chemisorbed O phases to bulk oxide phases may play an important role in oxidation catalysis [18]. There are numerous other examples of adsorbate-induced reconstruction of the surfaces (for example the lifting of the hex reconstruction on Pt(100) upon CO adsorption) that are beyond the direct simulation of DFT. Another more complex example is also shown in **Catalysis by Design**, where encapsulation of metal nanoparticles occurs under reaction conditions and affects the selectivity of the reaction. While DFT can be used *post priori* once these structures have been experimentally identified, currently it is difficult to predict these complex transitions *a priori*. Because of computational cost it is also difficult to explicitly simulate solvent-surface interactions, which are becoming of more interest with the convergence of homogeneous-heterogeneous and biological-heterogeneous convergence in the pursuit of highly tailored catalysts.

The workshop suggested encouraging researchers that can tackle the limitations of DFT through linking *ab initio* methods with methods that can access

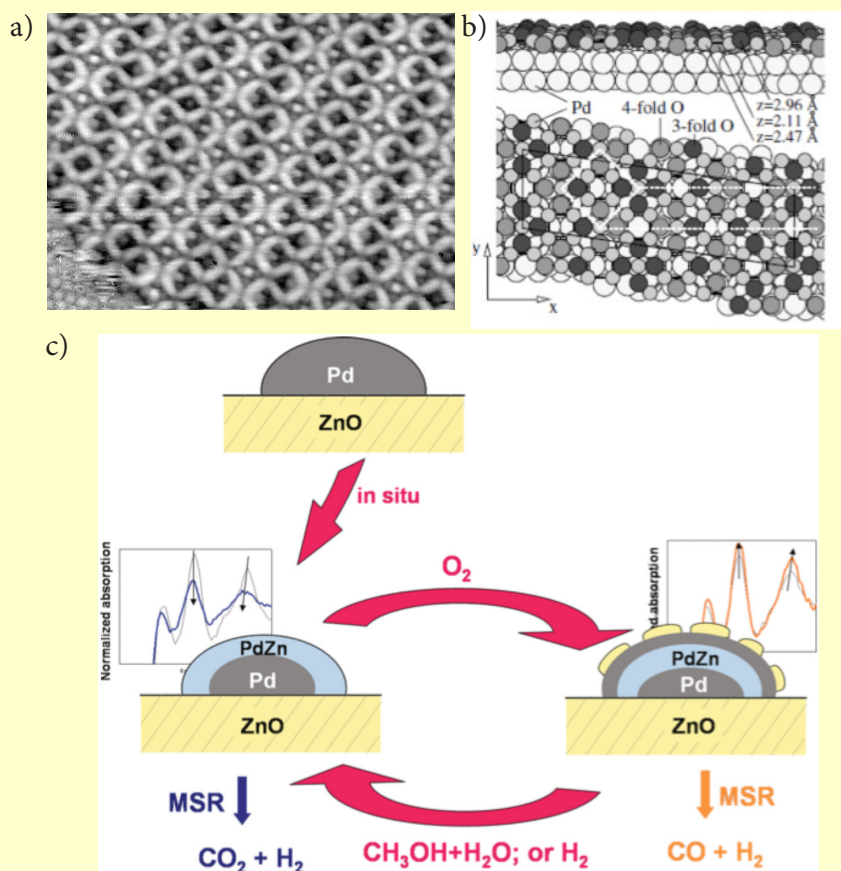


Figure 4. Breakout session of the photocatalysis and electrocatalysis working group.

experimental length and time scales of complex catalyst systems. Methods such as reactive potentials, QM/MM, kinetic Monte Carlo for reactive systems, and linking simulations at the atomic scale to the continuum scale (e.g., reactive computational fluid dynamics (CFD) simulations based on atomic-level

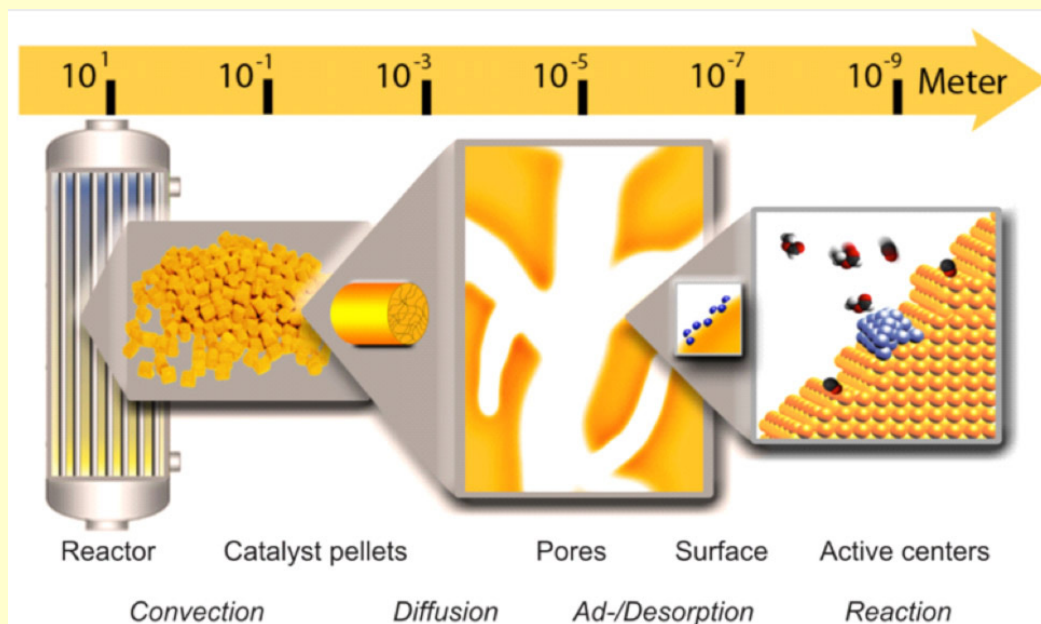
simulations of surface reactions) should be potential areas that can have a large impact on computational catalysis in the next decade. NSF Catalysis Division should promote the pursuit of novel methods that would allow for connecting the atomic-scale mechanisms occurring on surfaces and interfaces all the way to the reactor performance in a range of complex environments (see **Multiscale Simulation of Catalysis** [19]). The NSF Catalysis division is not appropriate for pure methods development (this belongs in the realm of NSF Chemical Theory, Models, and Computational Methods Division) but it should encourage the application of modeling methods beyond DFT that can tackle the challenges mentioned above. The cross-cutting workshop subgroup stressed that such modeling efforts should be driven by application to real-world problems, potentially through collaboration with experimentalists. The NSF Catalysis

Catalysis by Design



(a) STM image of the Pd surface oxide that forms on Pd(111) and (b) the DFT resolved minimum structure corresponding to the STM image of the Pd surface (from [17] Lundgren, Kresse *et al.*, *Physical Review Letters* 2002). (c) *In situ* EXAFS study shows that Pd/ZnO catalysts undergo complex encapsulation that is dependent on the reaction conditions. Furthermore, the selectivity of the methanol steam reforming reaction is sensitive to these changes (from [18] Föttinger *et al.*, 2011, *J. Phys. Chem. Lett.* **2**: 428-433).

Multiscale Simulation of Catalysis



Length scales involved in heterogeneous catalysis spanning meters to angstroms. Catalyst behavior is impacted by processes such as convection, diffusion, and surface reactions that can also span many orders of time scales. ([19] Figure provided by Professor Marcus Bäumer of Universität Bremen; composed by Marcus Bäumer and Arne Wittstock).

Division, therefore, has an opportunity to bridge the transition between method development and applications in the computational catalysis area, which in turn would ensure that the catalysis area has the well-developed tools to tackle the challenges in designing new catalysts for sustainable energy generation, storage, and use over the coming decades.

Conclusions

This section summarizes the conclusions of the workshop arrived at through the distillation of suggestions from the working group meetings and then refined through a discussion at the end of workshop, led by co-chairs [Figure 5], with input from all the attendees.

Federal catalysis agencies should focus on the fundamental understanding and prediction of catalytic chemical transformations which will

- lead to significant advances to address societal needs in a sustainable manner
- identify key classes of chemical transformations that can be addressed through catalysis; *e.g.*, C-H functionalization, removal of functionality from biomass (deoxygenation), sustainable synthesis of well-defined polymer architectures

- understand how to promote and control thermodynamically uphill processes
- characterize the active sites and underlying mechanisms for individual bond-breaking/formation steps
- construct model systems to elucidate mechanism and establish benchmarks for disentangling complex systems

Catalysis agencies should seek to understand the dynamic nature of catalysts addressing

- the design of resilient, self-repairing materials and molecules in order to extend catalyst lifetimes
- insights into the modes of catalyst deactivation
- *in situ* tools and studies to understand and capitalize on changes in structure, composition and molecular structure in catalysts of all types—heterogeneous, homogeneous, electrochemical, photochemical, and biological (enzyme) catalysts
- the development of new theoretical methods aimed at validated accuracy and their application to specific problems

Catalysis agencies should support activities that take a systems approach—designing a system of catalysts that allows for reactions that no individual catalyst



Figure 5. Professors Melanie S. Sanford, University of Michigan; Cynthia M. Friend, Harvard University; and Héctor D. Abruña, Cornell University, co-chairs of the workshop.

would effect including the design of

- tandem catalytic sequences to selectively enable multistep, complex transformations—focus on capturing and transforming unstable intermediates
- catalytic “assembly line”—enhance efficiency/selectivity of processes
- multifunctional, “Janus” (2-faced) catalysts for controlling selectivity and activity—example of acyl carrier proteins in enzyme catalysis or multifaceted nanoparticles

Catalysis agencies should also support the development of new sustainable catalysts and architectures which

- increase the efficiency of catalysts by exploiting architectures and dimensionality; *e.g.*, trapping precious materials catalytically species in nano- or meso-porous frameworks
- promote the design of selective active sites and assemblies of active sites with molecular-level precision
- leverage the cooperativity of active sites
- design new ligand structures that are robust to oxidizing and/or reducing conditions
- design catalysts based on earth-abundant metals
- develop new separation methodologies that will significantly aid in recycling precious catalysts in conjunction with other programs in the CHEM Division

Catalysis agencies should provide support for outreach and for a broader impact in society by

- training a diverse group of future leaders

- tapping into public interest in sustainability and develop courses for nonscientists that focus on sustainability
- working with University leaders to recognize the value of interdisciplinary and collaborative work that contributes to sustainability through catalysis; likely to lead to a more diverse faculty and student population

Catalysis agencies should establish mechanisms to promote collaboration in the catalysis community by

- making supplemental funding available for strategic collaborations; *e.g.*, a joint project between theorists and experimentalists focused on specific problems in catalysis; use of special techniques or tools to address a problem in catalysis—single molecule imaging, combinatorial catalysis screening, X-ray or optical probes of catalyst materials under reactions conditions
- supporting annual PI meetings of catalysis scientists across areas and scheduling these meetings in association with ACS meetings to enhance attendance
- supporting hands-on workshops for students, postdoctoral fellows, or other researchers for training and for fostering collaborations
- actively engaging industrial participants in these workshops and PI meetings to encourage partnerships and information exchange with the catalysis community

Finally, federal agencies should support instrumentation centers by

- identifying key instrumentation that is inaccessible in single-investigator laboratories and then fund a national network of Instrumentation Centers. Funding of ~\$20 M/Center would provide the necessary capabilities to the Center to support catalysis research—examples would be high throughput screening facilities, imaging (TEM, SEM, AFM, FIB), and chemical characterization (AP-XPS) Centers
- providing funding for technical staff and maintenance of facilities, for example, with support both through the NSF CHE Catalysis program or consider partnering with existing with NSF facilities networks, *e.g.*, the NNIN program [20]
- ensuring these national Centers incorporate data storage and mining to enhance capability for

directed and rapid design of catalytic materials and processes

Critical Directions

This section summarizes the critical directions that represent a consensus of the workshop attendees.

Direction 1. *Robust funding of catalysis is crucial to maintaining the nation's competitiveness. The workshop participants strongly endorsed catalysis funding reflect the full breadth of research areas represented in the workshop and focus on support of fundamental research.*

There are critical challenges in each of the areas of catalysis (homogeneous, heterogeneous and surface chemistry, bio-inspired, photo- and electrocatalysis) that need to be addressed. Support for experimental and computational efforts in all these areas as well as important synergies among them is vital to progress in the 21st century.

Support for fundamental research in catalysis will provide a new understanding of catalytic transformations, the important dynamical nature of catalysis, tandem or assembly line actions, and important new sustainable catalysis. More applied research also falls within the portfolios of other federal agency programs.

Direction 2. *Catalysis funding should support graduate student and postdoctoral fellowships that will allow researchers to gain experience across the areas of catalysis and provide supplemental funding to grants in the program to promote collaboration across the program.*

While the majority of funding from the federal agencies support single investigator awards, creation of supplemental funding for catalysis grantees would provide opportunities to explore synergies across different areas of catalysis. These supplementary awards can lead to important systems approaches that no individual catalysis would effect or joint projects between theorists and experimentalists. Support for graduate student fellowships would provide training in the important field at an early career stage while support through postdoctoral fellowships would also allow researchers with expertise in one area of catalysis to work in another discipline promoting diverse training across the field.

Direction 3. *An annual Catalysis Workshop should be held in conjunction with one of the American Chemical Society (ACS) national meetings to build*

stronger ties across the catalysis community.

An annual catalysis workshop, especially timed in association with the ACS meeting when many chemists are already planning to be in attendance, will help build the catalysis effort by providing exposure to the broader range of efforts in the federally supported catalysis portfolio. This would not only provide a showcase for the latest results but also foster new collaborations and synergies among scientists working in different areas of chemistry through the inclusion of interested researchers in catalysis, synthesis, and also with industrial scientists.

Direction 4. *The workshop attendees urged the funding by federal agencies of 1-3 Regional Instrumentation Centers (\$20 M capital investment, \$5 M/yr for operational support) that would provide the needed state-of-the-art instrumentation to support catalysis research as well as serve as a repository for the design of catalytic materials and processes for the nation.*

Much of the instrumentation to make progress in catalysis research is well beyond the scope of single-investigators. The establishment by federal agencies of 1-3 Instrumentation Centers as a network of essential mid-size facilities (e.g., high-throughput screening facilities, electron and atomic imaging, and chemical characterization) would be a key resource for catalysis research with a capital investment of \$20M per Center. Critical to the success of the Instrumentation Center network, however, is to provide funding of \$5M/year for technical staff members and the attendant instrumentation maintenance [20]. The operational support could be done through the NSF catalysis program or partnering with other existing NSF facilities such as the NNIN network for nanosciences (see Appendix IV). In addition, these national Centers should incorporate data storage and mining to enhance the capabilities for directed and rapid design of catalytic materials and processes [4].

Direction 5. *Catalysis program officers should work across divisions and directorates at their federal agencies to garner additional support for activities including graduate and postdoctoral fellowships or joint workshops.*

Given that catalysis plays such a vital role in many key processes, the workshop participants urged that catalysis program officers to work together across their respective divisions and directorates and as well

as synergistically with their wider agency initiatives like the Science, Engineering and Education for Sustainability (SEES) program at NSF. These broader and cross-cutting NSF programs are also an important opportunity for the catalysis program officers to help support the vital training through the postdoctoral fellowships and integrative joint meetings identified by the workshop participants.

References

1. Kapur, S.; Chen, A.; Cane, D.; Khosla, C., *PNAS*, **107**(51): 22066-22071, 2010 and Khosla, C. *et al.*, *Annu. Rev. Biochem* **76**: 195-221, 2007.
2. Crisci, A.J.; Tucker, M.H.; Dumesic, J.A.; Scott, S.L., "Acid-Functionalized SBA-15-Type Silica Catalysts for Carbohydrate Dehydration," *ACS Catalysis* **1**:719, 2011.
3. Barnett, S.; Goldberg, K.I.; Mayer, J.M., "Soluble Copper-Pyridine Water-Oxidation Electrocatalyst," *Nature Chem.* **4**: 498-502, 2012.
4. Materials Genome Initiative, Office of Science and Technology Policy, June 24, 2011, available from: http://www.whitehouse.gov/sites/default/files/microsites/ostp/materials_genome_initiative_final.pdf
5. Available from: http://nobelprize.org/nobel_prizes/chemistry/laureates/.
6. Committee on the Review of the Basic Energy Sciences, C.S.P., National Research Council *Catalysis for Energy: Fundamental Science and Long-Term Impacts of the U.S. Department of Energy, Basic Energy Science Catalysis Science Program*, 2009, National Academies Press.
7. Panel on New Directions in Catalytic Science and Technology, N.R.C., *Catalysis Looks to the Future*, 1992.
8. Committee on Benchmarking the Research Competitiveness of the United States in Chemistry, N.R.C., *The Future of U.S. Chemistry Research: Benchmarks and Challenges*, in *National Research Council Report*, 2007, National Academies Press.
9. Tao, F.; Grass, M.E.; Zhang, Y.; Burtcher, D.R.; Renas, J.R.; Liu, Z.; Chung, J.Y.; Mun, B.S.; Salmeron, M.; G.A. Somorjai, "Reaction-driven Restructuring of Rh-Pd and Pt-Pd Core-shell Nanoparticles," *Science* **322**: 932, 2008.
10. Dreher, S.D.; Dormer, P.G.; Sandrock, D.L.; Molander, G.A., *J. Am. Chem. Soc.* **130**: 9257, 2008.
11. McNally, A.; Prier, C.K.; MacMillan, D.W.C., *Science* **334**: 1114, 2011.
12. Dhamankar; Prather, K.L.J., "Microbial chemical factories: Recent advances in pathway engineering for synthesis of value added chemicals," *Curr. Opin. Struct. Biol.* **21**(4): 488-494, 2011: doi 10.1016/j.sbi.2011.05.0012011.
13. Prather, K.L.J.; Martin, C.H., "De novo biosynthetic pathways: rational design of microbial chemical factories," *Curr. Opin. Biotechnol.* **19**(5): 468-474, 2008: doi 10.1016/j.copbio.2008.07.009.
14. Moon, T.S.; Yoon, S.-H.; Lanza, A.M.; Roy-Mayhew, J.D.; Prather, K.L.J., "Production of glucaric acid from a synthetic pathway in recombinant *Escherichia coli*," *Appl. Environ. Microbiol.* **75**: 589-595, 2009: doi 10.1128/AEM.00973-08.
15. Atsumi, S.; Hanai, T.; Liao, J.C., "Non-fermentative pathways for synthesis of branched-chain higher alcohols as biofuels," *Nature* **451**(7174): 86-89, 2008: doi 10.1038/nature06450.
16. Yim, H. *et al.*, "Metabolic engineering of *Escherichia coli* for direct production of 1,4-butanediol," *Nature Chem. Biol.* **7**(7): 445-452, 2011: doi 10.1038/NCHEMBIO.580.
17. Lundgren, E.; Kresse, G.; Klein, C.; Borg, M.; Andersen, J.N.; De Santis, M.; Gauthier, Y.; Konvicka, C.; Schmid, M.; Varga, P., "Two-dimensional oxide on Pd(111)," *Phys. Rev. Lett.* **88**(24): 246103, 2002.
18. Föttinger, K.; van Bokhoven, J.A.; Nachtegaal, M.; Rupprechter, G., "Dynamic Structure of a Working Methanol Steam Reforming Catalyst: In Situ Quick EXAFS on Pd/ZnO Nanoparticles," *J. Phys. Chem. Lett.* **2**(5): 428-433, 2011.
19. Figure provided by Professor Marcus Bäumer of Universität Bremen; composed by Marcus Bäumer and Arne Wittstock.
20. Midsize Facilities: Infrastructure for Materials Research. 2005, National Academies Press, available from http://www.nap.edu/catalog.php?record_id=11336.

APPENDIX I: Attendees at the Workshop

Keynote Speakers

Frank J. DiSalvo, Cornell University
Matthew S. Platz, Director, Chemistry Division,
NSF
Helmut Schwarz, Technische Universität Berlin,
and President of the Alexander von Humboldt
Foundation

Main Speakers

Arvind Asthigiri, Ohio State University
Stefan Bernhard, Carnegie Mellon University
Juan M. Feliu, University of Alicante, Spain
Karen I. Goldberg, University of Washington
William A. Goddard III, California Institute of
Technology
Robert H. Grubbs, California Institute of
Technology
John F. Hartwig, University of California, Berkeley
Chaitan Khosla, Stanford University
Daniel G. Nocera, Massachusetts Institute of
Technology
Kristala Jones Prather, Massachusetts Institute of
Technology
Susannah Scott, University of California, Santa
Barbara
Gabor A. Somorjai, University of California,
Berkeley
Huimin Zhao, University of Illinois

Participants

Michelle C. Chang, University of California,
Berkeley
Donna A. Chen, University of South Carolina
Jeffrey Fosdick, Administration, Harvard
University
Robert L. Graham, Jr., Reporter, Harvard
University
Friederike Jentoft, University of Oklahoma
Anne McNeil, University of Michigan
Bruce A. Parkinson, University of Wyoming
Tomislav Rovis, Colorado State University
Keith J. Stevenson, University of Texas, Austin
Yi Tang, University of California, Los Angeles
Jason F. Weaver, University of Florida
Emily A. Weiss, Northwestern University
Mary Beth Williams, Pennsylvania State
University
Tehshik P. Yoon, University of Wisconsin

Discussion Groups

Heterogeneous Catalysis:

Donna A. Chen and Susannah Scott (*leaders*)
Friederike Jentoft, Gabor A. Somorjai, and Jason
F. Weaver

Homogeneous Catalysis:

John F. Hartwig and Tomislav Rovis (*leaders*)
Karen I. Goldberg, Robert H. Grubbs, Anne
McNeil, and Tehshik P. Yoon

Bio-Inspired Catalysis:

Chaitan Khosla and Kristala Jones Prather (*leaders*)
Michelle C. Chang and Yi Tang

Photo- and Electrochemical Catalysis:

Stephan Bernhard and Keith J. Stephenson (*leaders*)
William A. Goddard, Juan Feliu, Daniel G.
Nocera, and Emily A. Weiss

Cross-Cutting Activities and Computational Catalysis:

Bruce A. Parkinson and Huimin Zhao (*leaders*)
Arvind Asthigiri, John F. Hartwig, Frank J.
DiSalvo, and Helmut Schwarz

Members of NSF

Tyrone D. Mitchell, Program Director,
Environmental Chemical Sciences
Carlos A. Murillo, Program Director, Catalysis,
Instrumentation, and Cyber-enabled Chemistry
Matthew S. Platz, Director, Chemistry Division
Tong Ren, Program Director, Catalysis and
Chemical Synthesis

Co-Chairs

Héctor D. Abruña, Cornell University
Cynthia M. Friend, Harvard University
Melanie Sanford, University of Michigan

APPENDIX II: Workshop Program

NSF Chemical Catalysis Workshop

August 26–27, 2011, Denver, Colorado

Friday Evening, August 26, 2011:

- 4:30 pm Organizational Meeting of Co-PIs, Area Leaders and Breakout Session Scribes
5:00 pm Social Hour
Co-PIs:
Cynthia M. Friend, Professor of Chemistry, Harvard University
Hector D. Abruña, Cornell University
Melanie Sanford, University of Michigan
6:00 pm *Dinner*

Session 1: Opening Remarks, Introductions and Goals of Workshop

- 6:00 pm Mathew Platz, Director, Chemistry Division, NSF: “Catalysis”
6:30 pm Hector D. Abruña, Cynthia M. Friend, Melanie Sanford, “Introduction”
6:45 pm **Keynote Speaker:** Frank J. DiSalvo, Cornell University, “Sustainability: Humanity’s Ultimate Challenge”
7:15 pm **Keynote Speaker:** Helmut Schwartz, Technical University, Berlin, and President of the Alexander von Humboldt Foundation, “Catalysis Research in Germany — A Glimpse rather than a Survey”
7:45 pm Discussion
8:15 pm **Poster Session**

Saturday, August 27, 2011

- 7:00 am *Continental Breakfast*

Session 2: Heterogeneous Catalysis and Surface Chemistry (Moderator: C. M. Friend)

- 8:00 am Gabor A. Somorjai, University of California, Berkeley, “The Rapid Evolution of Molecular Catalysis: Science from the Perspective of Surface Science”
8:30 am Susannah Scott, University of California Santa Barbara, “Heterogeneous Catalysis for Sustainability”
8:45 am Arvind Asthigiri, Ohio State University, “Computational Catalysis”

Session 3: Homogeneous Catalysis and Organic Synthesis (Moderator: M. Sanford)

- 9:00 am Robert H. Grubbs, California Tech, “Homogeneous Catalysts: Green Chemistry, Metathesis”
9:30 am John F. Hartwig, University of California, Berkeley, “The State of Catalyst Design: Successes and Future Challenges for Homogeneous Catalysis”
9:45 am Karen I. Goldberg, University of Washington, “Homogeneous Catalysis: Essential for Sustainability”
10:00 am *Coffee Break*

Session 4: Bio-inspired Catalysis (Moderator: M. Sanford)

- 10:15 am Chaitin Khosla, Stanford University, “Biocatalysis”
10:45 am Huimin Zhao, University of Illinois, “Opportunities and Challenges in Biocatalysis”
11:00 am Kristala Jones Prather, Massachusetts Institute of Technology, “Challenges and Opportunities in Bio-based Synthesis”

Session 5: Photocatalysis and Electrocatalysis (Moderator: H. Abruña)

- 11:15 am William A. Goddard III, California Tech, “The Role of Theory in Catalysis and Sustainability”
11:45 am Dan G. Nocera, Massachusetts Institute of Technology, “Energy (Fuels) Catalysis”
12:15 pm Juan Feliu, University of Alicante, “Electrocatalysis: Surface Reactivity in Condensed Media”
12:45 pm Stefan Bernhard, Carnegie Mellon, “Solar Fuels: Thermodynamics, Tactics, and Recent Results”
1:00-2:00 pm Working Lunch with Directed Discussion Cutting across Areas
Breakout Session I:
2:00 pm Report back from Breakout
3:00 pm *Break*
3:15 pm Breakout Session II: Refinement of Area Reports
4:00 pm Report back from Breakout Session
5:00–6:30 pm *Co-PIs prepare for Plenary Report*
5:30-6:00 pm Social Hour and Informal Discussion
6:30-8:00 pm *Working Dinner with Report back*
8:00 pm Summary and Overview
8:30 pm Adjournment of General Meeting

APPENDIX III: Poster Session

Friday August 26, 2011

Heterogeneous Catalysis:

Donna A. Chen, University of South Carolina

Friederike Jentoft, University of Oklahoma

Jason F. Weaver, University of Florida

Homogeneous Catalysis:

Anne McNeil, University of Michigan

Tomislav Rovis, Colorado State University

Tehshik P. Yoon, University of Wisconsin

Photo- and Electrochemical Catalysis:

Emily A. Weiss, Northwestern University

Bruce A. Parkinson, University of Wyoming

Mary Beth Williams, Pennsylvania State University

Keith J. Stevenson, University of Texas at Austin

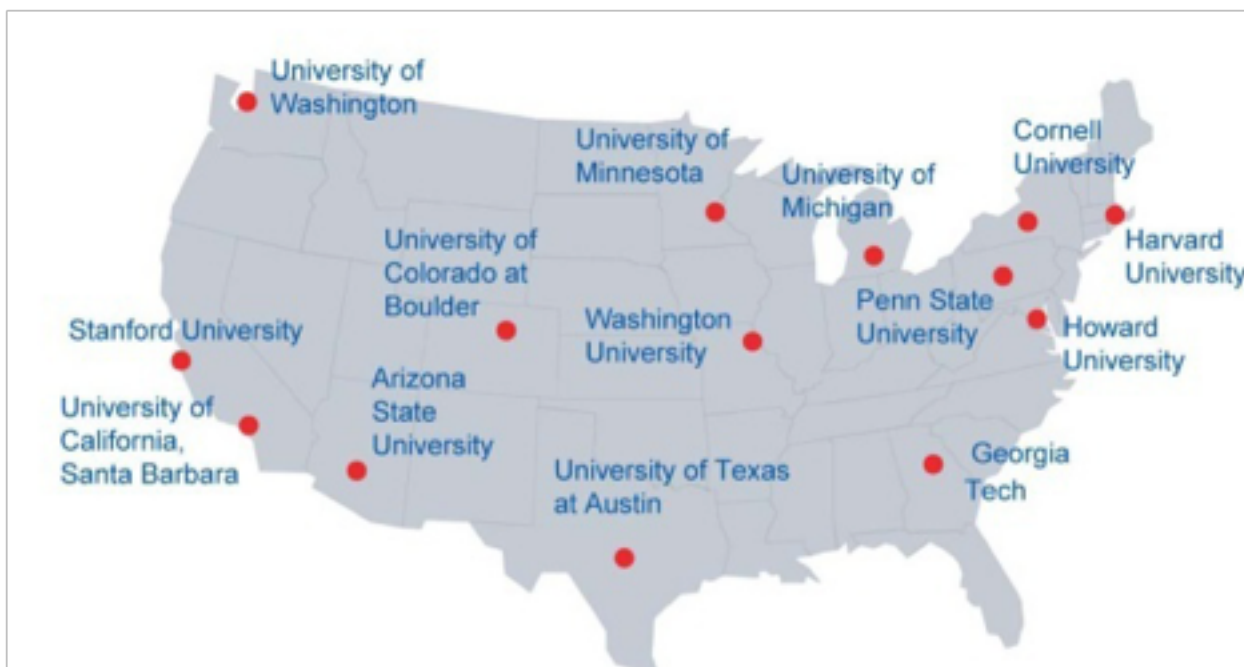
Biocatalysis:

Michelle C. Chang, University of California at Berkeley

Yi Tang, University of California at Los Angeles

APPENDIX IV: National Nanotechnology Infrastructure Network (NNIN)

During the past decade, a substantial investment by the multiagency National Nanotechnology Initiative has been made in nanotechnology centers. The National Nanotechnology Infrastructure Network (NNIN) was established to provide mid-size facilities for fabrication and characterization of nanomaterials that were distinct from the capabilities of large-scale facilities such as photon or neutron sources. The NNIN is a collective of fourteen university-based facilities to enable advances in nanoscale science, engineering, and technology with nearly 150 full-time technical staff providing training to its over 5,000 annual users. Through its regional distribution, the NNIN serves researchers at many institutions that face challenges associated with the availability of such instrumentation crucial to the fabrication or growth of new or high-quality nanomaterials. In addition, the NNIN offers computational and theoretical tools for understanding the behavior of nanostructures and devices.



Institutions of the National Nanotechnology Infrastructure Network, 2010-2011