National Science Foundation Workshop
on
Future Directions in Catalysis:
Structures that Function at the Nanoscale

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NSF Headquarters
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NSF Workshop on Future Directions in Catalysis: Structures that Function at the Nanoscale

Background

Recent advances in the synthetic methodologies used to control nanometer-sized assembly, analytical methodologies employed to identify and probe structure at the nanometer length scale, and predictive capabilities used to provide guiding principles of nanometer scale structure/property relationships suggest that the synthesis of new catalysts with unprecedented control of the structure at the nanometer length scale is likely in the near future. Additionally, nanofabrication methods have developed to the point where size, shape and functionality of materials can be controlled at the length scale of tens of nanometers. Thus, catalytic systems with control over multiple length scales spanning the atomic, molecular and nanometer scales are on the near horizon. This unprecedented control of structure and composition will lead to unprecedented control over reaction efficiencies and selectivities.

Objectives and Description of Workshop

The purpose of the workshop was to bring together a leading group of engineers and scientists from academia, industry and government agencies to focus on the future directions of catalysis. The workshop objectives were to:

* Assess the state-of-the-art in synthetic methodologies aimed at specifically creating organization at the nanometer length scale for the preparation of catalytic materials for the exploitation of catalysis to create other materials.
* Assess the state-of-the-art analytical methodologies as they apply to the study of reacting materials in order to address whether they can provide reliable information sufficient to define structure/function at the nanometer length scale.
* Assess the state-of-the-art computational methodologies regarding their ability to provide quantitative descriptions and accurate predictions of systems that have nanometer scale organization.
* Provide visionary statements as to what future synthetic methodologies might be, what nanometer scale architectures might arise from these assembly strategies, and what will be necessary to achieve the creation and exploitation of these new materials in future technologies.
* Provide guiding statements for educational and training needs.
* Provide guiding statements for interactions with other national initiatives such as the National Nanotechnology Initiative (NNI).

The workshop was held at NSF Headquarters in Arlington, VA, on June 19 and 20, 2003. A website at **http://cheme.caltech.edu/nsfcatworkshop/** contains all reporting documents and presentations from the workshop.

Grand Challenge

The overall guiding theme and grand challenge that emerged from the workshop was:

* ***To control the composition and structure of catalytic materials over length scales from 1 nanometer to 1 micron to provide catalytic materials that accurately and efficiently control reaction pathways.***

The workshop participants endorsed the concept that catalysts are nanoscaled engines, and in order to have these engines "power" future (nano)technology, control of their composition and structure over length scales from 1 nanometer to 1 micron will be necessary.

<u>Major Outcomes</u>

Assembly (all points to be addressed in the next 10-15 years)

* In order to design and control the assembly of structures over multiple length scales, it will be necessary develop a repertoire of inorganic and organic-inorganic hybrid, nanometer-sized, synthetic building units that can be assembled into well defined architectures.
* Effective design of these assemblies will also require a fundamental understanding of how collective behavior, e.g., multitudes of weak forces, functions in the assembly of structures to create high precision like what is currently achievable with (bio)organic assembly.
* Self-assembly in both vapor and condensed phases provides a promising synthetic pathway to these assemblies, but achieving controlled synthesis using these methodologies will necessitate a fundamental understanding of the nucleation and growth processes and their dynamics.
* The design and creation of individual catalytic "modules" that operate properly will only be accomplished through a better understanding of how to use kinetically controlled pathways to achieve metastable states and how to stabilize these metastable states at reaction conditions.
* Design and synthesis of multicomponent catalytic systems that integrate multiple reaction pathways and types of reactions will require the development of methods for incorporating the individual catalytic "modules" into complex functioning assemblies. Nanofabrication methods have developed to the point where the size, shape and functionality of materials can be controlled at length scales ranging from 50 nm to 1 micron. These methods should be exploited to create new catalytic systems where the reactive centers are placed within nanostructures specifically designed for the desired chemical conversions. Nanofabrication tools indicating optical and e-beam lithography, imprinting, reactive ion etching and chemical vapor deposition provide exciting opportunities for synthesizing new catalytic materials.

Characterization

* Although numerous facilities are available within the US for characterizing catalytic materials, there remains a need for facilities that are beyond the cost and support personnel structures typical of educational institutions. Specifically, national facilities and support personnel are needed to allow multi-investigators to:
    * facilitate measurements of both average properties and single active centers at reaction conditions using techniques such as *in situ* transmission and scanning

electron microscopies with sample transfer between instruments. (Next 5-10 years).
    * enable measurements of the same material over multiple length scales using techniques such as simultaneous, *in situ* wide and small angle X-ray scattering. (Next 5-10 years).
* Although exemplary cases of *in situ* characterization methodologies have been reported, the consensus is that advancements that extend the limits of temperature, pressure and resolution both in space and time of current spectroscopies will be necessary to meet the grand challenge. Particular emphasis should be placed on efforts involving measurements in reaction environments containing potentially corrosive reagents. (Next 10-15 years).
* The next generation of instruments and characterization methods will require interdisciplinary efforts for the development of the instruments and the interpretation of the data acquired from them. Avenues must be provided for theorists and modelers to work closely with instrumentalists to develop accurate, nanoscale characterization methodologies. (Next 10-15 years).

Computation and Modeling

* While numerous advances in theory, modeling and simulation have reached the stage where they can be used to determine and predict chemical and physical properties of some nanoscale systems, deeper understanding and more complete descriptions of complex reactions and collective behavior including self-assembly in solution will require the development of new theories (Next 10-15 years).
* Since catalyst assembly and function can occur over many time scales, e.g., femtoseconds to hours, new methodologies that are capable of spanning multiple time scales will be necessary to meet the grand challenge. (Next 5-10 years).
* Well-defined experiments are required in order to generate data useful for theory validation and database construction. Avenues need to be provided for theorists and modelers to work closely with experimentalists to design and conduct well-defined experiments that can provide meaningful data for theory validation and knowledge accumulation in the form of databases. (Next 5-10 years).
* There is a need for more meaningful predictive capabilities, e.g., descriptions of assembly pathways that occur in liquids. These needs necessitate the development of more accurate methods and models. (Next 10-15 years).

Education and Training Needs

Advances in nanoscience and engineering due to innovative research in catalysis will provide important new opportunities for workforce expansion within specific emerging technical areas. Anticipation of the appropriate time-frame for the development of enhanced human resources with the prerequisite skills is necessary. Significantly increased needs could be expected within five to ten years due to the direct application of nanoscale catalysis for energy and chemicals production. Even larger demands are likely for a long-term economic expansion that would utilize catalysis to produce nanomaterials, integrated devices, or value-added consumer products. Recent declines in the number of US students engaged in graduate engineering and science education have been disproportionately reflected in catalysis research. Nanoscience and engineering education provides an important opportunity to attract new students at the undergraduate and graduate levels due to the cutting-edge nature of the research and the promising technological applications. Important opportunities also exist for enriching university curricula and for augmenting existing K-12 programs within the National Nanotechnology Initiative. Development of a diverse group of talented students is essential for all programs under this initiative. Nanoscience and engineering education is inherently interdisciplinary, and creation of integrated research teams and networks for innovative catalysis research is encouraged. The availability of advanced characterization facilities for training the next generation of catalysis researchers is also a key workforce concern.