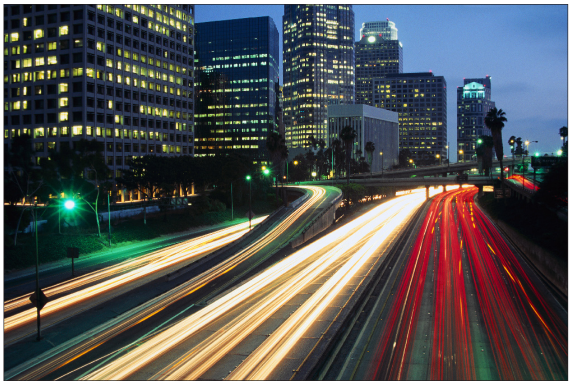
Catalysis for Energy:

Fundamental Science and Long-term Impacts of the U.S. Department of Energy Basic Energy Sciences Catalysis Science Program

Catalysis is essential to our ability to control chemical reactions, and therefore integral to current and future energy solutions. At the request of the U.S. Department of Energy (DOE), this report presents an in-depth analysis of the investment in catalysis basic research by DOE's Office of Basic Energy Sciences Catalysis Science Program. The report finds that investments in the program have been well directed, have led to a greater understanding of fundamental catalytic processes, and have contributed to long-term national energy goals. The report concludes that the program's succesful model for funding single investigator and small group grants should continue, with some specific recommended changes in the types of studies pursued.



Energy —its production, storage, and utilization—constitutes one of the most important and challenging issues in the United States. To achieve its mission to advance the national, economic, and energy security of the United States, DOE supports basic physical-science research that focuses on energy-related issues. One of the most important areas is the study of catalysis, the process by which a substance (a catalyst) increases the rate of a chemical reaction. Catalysts are essential to energy transformations, and, thus, they are crucial to the development of current and future energy technologies.

DOE's Office of Basic Energy Sciences Catalysis Science Program is the primary funder of basic research on catalysis in the United States. The program has supported many well-established researchers who are world leaders in catalysis science. It has also supported many new researchers, who have largely entered the program recently through special initiatives, such as the Catalysis Science Initiative and the Hydrogen Fuel Initiative. The program has and should continue to play a key role in meeting national energy needs.

This report, which was produced at DOE's request, presents an in-depth analysis of the investment in catalysis basic research by the Catalysis Science Program. After careful review of the research portfolio (grant titles, abstracts, individual researchers), especially for the fiscal years 1999 to 2007, the report concludes that Office of Basic Energy Science has done well with its investments in catalysis basic research through the Catalysis Science Program. For example, the potential of biomass as an alternative source of energy has opened up a field of research that may have a substantial impact on the advancement of science and on progress

Meeting Energy Goals Through Catalysis

Catalysis is central to many exciting frontiers in producing and saving energy, for example:

Fuel Production:

- Converting biomass to liquid fuels
- Utilizing water as a source of hydrogen fuel

Chemical Production:

- Converting nonfossil fuel resources to chemicals
- Providing new energy efficient routes to chemical processing

Environmental Protection:

- Capturing emissions with greater efficiency and selectivity
- Converting pollutants to fuels and chemicals

toward meeting the nation's energy goals. Within the program's grant portfolio, J. Dumesic and colleagues have made a number of discoveries that were inspired by initial work that dealt with the selectivity for cleavage of C-O versus C-C bonds in oxygenated hydrocarbon intermediates on metal surfaces. This work has led to the recent success of a promising biorefinery concept.

The report attributes the program's success to key management decisions over the past eight years that have led to a current funding distribution that advances catalysis science in general and keeps the development of energy-related technologies as a long-term goal. The DOE Catalysis Science Initiative (CSI), which began in 2003 as a mechanism to encourage "high-risk, long-term, multi-investigator, multidisciplinary research on the science of catalysis," has been a particularly effective mechanism for bringing to the program new funds, new researchers, and innovative research topics. However, there are variations in the quality and relevance of the research in the program's portfolio, as summarized in the report's main findings and recommendations below.

Overview of the Catalysis Science Program

Since 1999, the Catalysis Science Program has sponsored more than 1,000 catalysis basic research grants at universities and national laboratories (Figure 1). For fiscal year (FY) 2007, the program was funded at approximately $38 million (3 percent of the BES budget). The program currently funds 170 principal investigators in 78 institutions. According to demographic information collected by the committee, the typical principal investigator being funded during fiscal years 1999 to 2007 was a full professor who had received a Ph.D. approximately 20 years earlier.

For convenience in evaluating the program, this report groups the Catalysis Science Program portfolio by the two main types of catalysis:

- **Heterogeneous catalysis**, the catalyst (typically a solid) is in a different phase from the liquid or gaseous reactants.
- **Homogeneous catalysis**, the catalyst is in the same phase (typically liquid) as the reactants.

It should be noted, however, that researchers are increasingly crossing the traditional barriers between heterogeneous and heterogeneous catalysis, blurring the distinction between the two, which the committee views as a definite positive development.

The grants in the Catalysis Science Program portfolio are distributed among individual researchers and small groups and cover a variety of research areas. Grants for research in heterogeneous catalysis include nanoscience, surface science, and theory and have averaged 70 percent of the program's portfolio. Grants for research in homogeneous catalysis include biocatalysis and have averaged 30 percent of the portfolio.

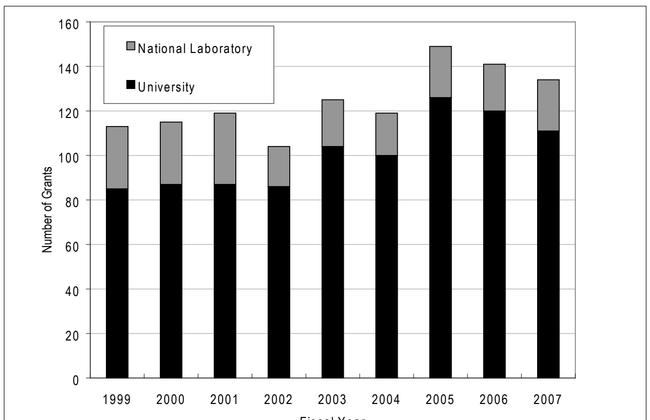


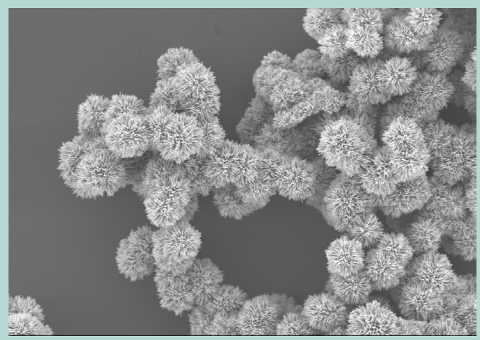
Figure 1 Catalysis basic research grants funded by DOE, FYs 1999-2007.
SOURCE: U.S. Department of Energy, Office of Basic Energy Sciences, Catalysis Science Program

SELECTED PROGRAM ACCOMPLISHMENTS:
Examples of Impact on Fundamental Science and Future Contributions to National Energy Goals

For the purposes of this study, the committee defined the fundamental science of catalysis as the general understanding of or insight into a catalysis system or a material that is fundamental enough to be applied to more than one specific catalyst. Additionally, the committee identified the national energy goals to be the improved production and use of current and future energy sources. Examples of areas where the Catalysis Science Program has had a significant impact on fundamental science or has made contributions to meeting national energy goals are provided below and in Chapter 5.

Modeling Catalytic Structures and Their Reaction Environment
By funding the development of computation methods for the analysis of heterogeneous catalysis for the past 10 years, the Catalysis Science Program has been the main contributor to the growth of theoretical understanding and modeling of surface catalytic structures. As a result, it is now possible to calculate activation energies of basic surface reactions to better understand the reactivity of various catalysts. For instance, see the work of the principal investigators M. Barteau, M. Mavrikakis, and M. Neurock.

Nanostructured Metal Oxides
During the past few years, catalysis scientists have dramatically improved their ability to design and synthesize inorganic sites with controlled size, atomic connectivity, and hybridization with either organic or other inorganic superstructures. The resulting materials contain chemical functions and physical properties that can be tuned for energy conversion, petrochemical synthesis, and environmental reactions. Several of the groups that have been funded by the Catalysis Science Program have made contributions to this area of fundamental science, such as principal investigators A. Bell, V. Guliants, J. Hrbek, E. Iglesia, C. Peden, S. Suib, and I.Wachs.


Source: S. Suib

Single-Site Polymerization Catalysts
Fundamental research by principal investigator J. Bercaw and colleagues, and expanded upon by other researchers, has resulted in the development of highly active single-site polymerization catalysts that are now used by U.S. industry to produce more than 2 billion pounds of polyolefins polymers a year. The new polymerization processes are more efficient, use less energy, and require less capital than prior technology, which has impacted polymer production around the world.

Recommendations

The Catalysis Science Program should continue its current approach to funding decisions. Multi-investigator and interdisciplinary programs such as the Catalysis Science Initiative should remain a part of the portfolio, but future teams might benefit from the inclusion of more homogeneous catalysis and biocatalysis researchers that are interested in energy solutions. The program should utilize future funding initiatives as a mechanism to maintain the balance of experienced and new researchers in the program and to explore new approaches to carrying out research.

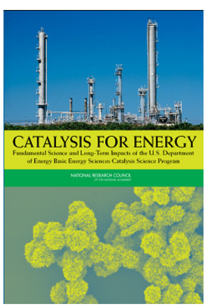
Influences on the Portfolio

The Catalysis Science Program should continue to broaden participation in its contractor meetings and other activities. Non-DOE sponsored workshop organizers and grantees funded by other Office of Basic Energy Sciences programs should be invited to attend the Catalysis Science Program's activities to provide a more diverse influence on the portfolio. This is particularly important in the development of research directions that will have a long-term impact on the program.

Principal Investigators
The Catalysis Science Program should continue on its current path of maintaining support for productive, long-term researchers and of recruiting new researchers. The program also must ensure that the best researchers are identified and supported—this is especially important in heterogeneous catalysis, because program funding is essential to the success of a heterogeneous catalysis researcher (see Chapter 3). The balance of funding for individual investigators and small groups should also be maintained.

Heterogeneous Catalysis
The distribution of grants in the heterogeneous catalysis portfolio should be changed slightly. Studies on high surface area catalysts, surface science, nanoscience, and electrocatalysis should be maintained, but there should be a stronger emphasis on studies that explore catalyst design and new synthesis methods, unique reactor systems, unique characterization techniques, and completely new chemical reactions. Support for the development of theoretical methods also should feature more prominently in the portfolio.

Homogeneous Catalysis
A balanced homogeneous catalysis portfolio should extend beyond individual mechanistic steps to include greater development of new catalytic systems and reactions. The portfolio can be improved by pursuing opportunities to work more effectively with carbon-hydrogen bonds (C-H bond functionalization), new approaches to transition-metal catalysis, and electrochemical catalysis (small molecule homogeneous catalysts supported on electrodes). In addition, there should be a greater emphasis on reducing highly oxidized compounds such as bioderived materials into fuels and feedstocks, and on bioinspired catalytic processes.



Committee on the Review of the Basic Energy Sciences Catalysis Program: Nancy B. Jackson, *(Co-chair)*, Sandia National Laboratory; **Jens K. Nørskov**, *(Co-Chair)*, Technical University of Denmark; **Mark A. Barteau**, University of Delaware; **Mark Cardillo**, The Camille and Henry Dreyfus Foundation, Inc.; **Marcetta Y. Darensbourg**, Texas A&M University; **Anne M. Gaffney**, Lummus Technology; **Vernon Gibson**, Imperial College, UK; **Sossina Haile**, California Institute of Technology; **Masatake Haruta**, Tokyo Metropolitan University; **Nenad Markovic**, Argonne National Laboratory; **Thomas A. Moore**, Arizona State University; **Brenden D. Murray**, Shell Oil Company; **James C. Stevens**, The Dow Chemical Company; **Barry Trost**, Stanford University; **Tina Masciangioli (***Study Director***)**, National Research Council.

The National Academies appointed the above committee of experts to address the specific task requested by the sponsor. The members volunteered their time for this activity; their report is peer-reviewed and the final product signed off by both the committee members and the National Academies. This report brief was prepared by the National Research Council based on the committee's report.

EXPERT CONSENSUS REPORT

For more information, contact the BCST at (202)334-2156 or visit http://dels.nas.edu/bcst/. Copies of *Catalysis for Energy: Fundamental Science and Long-Term Impacts of the U.S. Department of Energy Basic Sciences Catalysis Science Program* are available from the National Academies Press, 500 Fifth Street, NW, Washington, D.C. 20001; (800) 624-6242; www.nap.edu.