Recommendations for a National Catalysis Research Institute

Advanced Resources for Catalysis Science

Summary of the Workshop

held September 21-22, 2004
Pacific Northwest National Laboratory
Richland, Washington 99352

Catalysis is one of the most valuable contributors to our economy and historically an area where the United States has enjoyed, but is now losing, international leadership. While other countries are stepping up their work in this area, support for advanced catalysis research and development in the U.S. has diminished. Yet, more than ever, innovative and improved catalyst technologies are imperative for new energy production processes to ease our dependence on imported resources, for new energy-efficient and environmentally benign chemical production processes, and for new emission reduction technologies to minimize the environmental impact of an active and growing economy.

Addressing growing concerns about the future direction of U.S. catalysis science, experts from the catalysis community met at a workshop to determine and recommend advanced resources needed to meet the grand challenges for catalysis research and development. The workshop's primary conclusion: To recapture our position as the leader in catalysis innovation and practice, and promote crucial breakthroughs, we must **establish one or more well-funded and well-equipped National Catalysis Research Institutes competitively selected, centered in the national laboratories and, by charter, networked to other national laboratories, universities, and industry. The Institute(s) will be the center of a National Collaboratory that gives catalysis researchers access to the most advanced techniques available in the scientific enterprise.**

The importance of catalysis to our energy, economic, and environmental security cannot be overemphasized. Catalysis is a vital part of our core industrial infrastructure, as it is integral to chemical processing and petroleum refining, and is critical to proposed advances needed to secure a sustainable energy future. Advances in catalysis could reduce our need for foreign oil by making better use of domestic carbon resources, for example, allowing cost-effective and zero-emission conversion of coal into transportation fuels. No matter what energy sources are being considered (oil, natural gas, coal, biomass, solar, or nuclear based), a clean, sustainable energy future will involve catalysis to improve energy efficiency and storage and use options, and to mitigate environmental impacts.

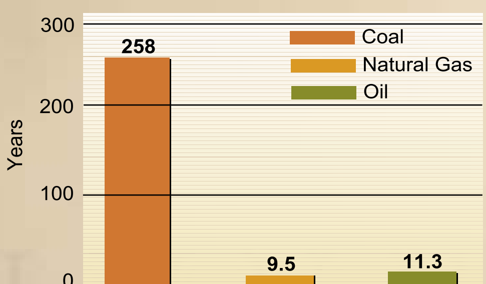
Recent revolutionary advances in nanotechnology and high-performance computing are enabling the breakthroughs in catalysis science and technology essential for a secure energy future. Thus, the time is right for substantially increased investments in catalysis science and technology.

Catalysis will help build a clean, sustainable energy future.

Advances in Catalysis Are Essential for Energy, Economic, and Environmental Security

While catalysis is considered a critical underpinning science for technologies relevant to our energy, economic, and environmental security, the United States, arguably, is no longer at the vanguard of cutting-edge work in this area. At the same time, the European Union, Japan, and other countries are pursuing catalysis as a matter of policy linked to their economic development. These policies are being promulgated through highly visible "flagship" centers devoted to catalysis science, which provide long-term, focused support for coordinated, multi-investigator, multi-disciplinary activity spanning the range of catalysis research and development. These organizational structures support a coherent integration of academic, industrial, and national research resources and efforts. There are no comparably organized and funded entities in the U.S. dedicated to catalysis research.

While incremental improvements to catalytic processes are leading to better control of desired chemical transformations with fewer undesirable side-products, these developments alone are not enough. Instead, revolutionary breakthroughs must be achieved to fully realize the needed advancements:



U.S. Fossil Fuel Reserve/Production Ratios – at current production levels, known U.S. coal reserves would last over 250 years.

Source: BP Statistical Review of World Energy 2004

- breakthroughs in photocatalysis to successfully and economically use solar energy to convert water into oxygen and hydrogen—a very clean-burning fuel.
- breakthroughs in interfacial electrocatalysis to realize, with competitive economics, the efficiency potentially attainable with fuel cells—devices that directly convert energy stored in molecules, like hydrogen, into electrical energy.
- breakthroughs in the gasification and conversion of coal into transportation fuels.
- breakthroughs in the catalytic conversion of biomass to more useful products, e.g., cellulose to glucose, to economically utilize the chemical energy stored in this renewable resource.
- breakthroughs in the development of catalysts that operate in aqueous media to fully enable the promise of "green chemistry."
- breakthroughs in the construction of nanoscale multi-component catalysts organized in mesostructures as viable alternatives to expensive and supply-limited precious metal catalysts.

Workshops Explore Future Needs of Catalysis Science and Technology

The economic and scientific considerations that underscore the significance of catalysis science and technologies—and the opportunities for catalysis scientists and engineers to help achieve a secure energy future—have been considered in great detail in recent workshops and reports (see Sources listed below). In May 2002, the U.S. Department of Energy's Office of Science, Basic Energy Sciences Advisory Committee (BESAC) sponsored the workshop "Opportunities for Catalysis Science in the 21st Century." The grand challenge emerging from that workshop was the need "to understand how to design catalyst structures to control catalytic activity and selectivity." The resultant report, along with others, recognizes the inherent complexity of catalytic phenomena, a complexity making interdisciplinary collaboration all the more important for expediently advancing catalysis science and technology. The prevailing theme in these reports is consistent: advances in experimentation, computation, and theory—especially those that allow the structural and chemical properties of materials to be tailored, tuned, and designed at the nanoscale—provide a unique collective opportunity for revolutionizing this field.

Building on prior observations and recommendations, the **Advanced Resources for Catalysis Science Workshop** convened September 21-22, 2004, at Pacific Northwest National Laboratory in Richland, Washington, to:

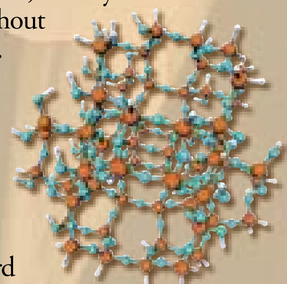
- define the specific state-of-the-art and next-generation tools for advancing the fields of catalysis science and engineering, and
- identify how best to ensure these tools are widely available to the catalysis research community.

The economic contribution of catalysis is as remarkable as the phenomenon itself. Approximately one third of material gross national product in the U.S. involves a catalytic process somewhere in the production chain. Confining analysis to the chemical industry, the proportion of processes using catalysts is 80% and increasing...

E Fontes & P Bosander. "Process Catalysis." *Chemistry & Industry,* January 21, 2002

Representing a broad spectrum, 27 experts from national laboratories, industry, and universities participated. The workshop comprised five plenary presentations addressing the current state of the science and the challenges, and four breakout sessions on specific advanced resource needs for catalysis research and development:

- **Catalyst Design, Synthesis, and Characterization** – The emerging experimental and computational tools of nanoscience, when integrated and focused, will enable ground-breaking scientific advances in catalyst design, synthesis, and characterization. These new tools will allow synthesis of catalysts with atom-by-atom precision and enable unprecedented control of the specificity and selectivity of chemical transformations. Enabling these scientific advances has the potential to revolutionize our ability to address the grand challenge for 21st Century catalysis—understanding how to design catalyst structures to control catalytic activity and selectivity.
- **Reaction Dynamics and Operando Characterization** – Designing new catalysts requires detailed information concerning the individual steps that determine rates of reaction, in particular, information on which steps are "rate-limiting." With this information, a catalyst can be structured to facilitate these steps without a negative impact on other elementary steps. To accomplish these objectives, tools must be available that can provide nanoscale spatial and femto- to milli-second time resolution measurements during actual catalyst operation, i.e., so-called "operando" conditions.



- **High-Throughput Methods** – A shift toward high-throughput "combinatorial" methods is changing the way catalysts are discovered, characterized, and tested. The technology is based on the use of robotics for both efficient synthesis and analytic evaluation of performance, coupled with data-intensive computing to enable the rapid discovery of promising new catalytic materials. To make a scientific impact on catalysis, combinatorial methods must also be utilized for fundamental studies.
- **Theory and Computation** – Revolutionary advances in high-performance computing hardware, theory development, and software, when benchmarked with detailed experimental results, allow realistic catalyst systems and processes to be simulated and modeled. These new tools enhance our understanding of known systems and processes by helping to interpret experimental results. They also can be used to enable the design of new catalytic materials and processes. Furthermore, simulation allows researchers to explore temporal and spatial domains that are not accessible by current experimental methods.

Recommendations from the Advanced Resources for Catalysis Science Workshop

The overriding recommendation, endorsed by all participants in the **Advanced Resources for Catalysis Science Workshop**, was the need to establish one or more well-funded and well-equipped National Catalysis Research Institutes (NCRIs) competitively selected, centered in the national laboratories and, by charter, networked to other national laboratories, universities, and industry. The NCRI(s) would provide, in centralized physical locations, tools dedicated to catalysis science that are too complex or too expensive for a single investigator or institution to support. This networked center(s) would facilitate high-risk, long-term, multi-investigator, multi-disciplinary research activities addressing specified challenges and needed breakthroughs.

Additional recommendations include the following:

- Specific suites of tools dedicated solely to catalysis research are required, including suites of "operando" experimental capabilities; a suite of computational tools for structural, dynamic, and microkinetic modeling of catalytic reaction systems; a suite of high-throughput combinatorial catalytic reaction tools; and an integrated suite of experimental tools dedicated to "operando" study of catalytic systems at one or more of the nation's third-generation synchrotron light sources. A key component is the availability of a "critical-mass" of experts in these areas whose focus is collaborative catalysis research.

Cutting-edge computational tools are fundamental to catalysis breakthroughs.

- The NCRI(s) should also focus on need-based development of new experimental and computational tools for the catalysis community.
- The NCRI(s) should have evolving, well-defined, long-term research agendas selected for scientific importance and potential impact, consisting of a closely integrated group of collaborators with appropriate expertise to address the interdisciplinary research themes.
- To encourage and strengthen university, particularly student, involvement and increase the participation of industrial users from throughout the country, the NCRI(s) should include a prominent virtual component. The NCRI(s) would receive sufficient support for amplifying, integrating, and accelerating the research of individual scientists at the Institute itself and at institutions participating in the virtual collaboratory.

Excerpt from *Opportunities for Catalysis Science in the 21st Century*, May 2002:

In his address to the 2002 meeting of the American Association for the Advancement of Science, Jack Marburger, the President's Science Advisor, spoke of the revolution that will result from our emerging ability to achieve an atom-by-atom understanding of matter and the subsequent unprecedented ability to design and construct new materials with properties that are not found in nature.

"The revolution I am describing," he said, "is one in which the notion that everything is made of atoms finally becomes operational.… We can actually see how the machinery of life functions, atom by atom. We can actually build atomic-scale structures that interact with biological or inorganic systems and alter their functions. We can design new tiny objects 'from scratch' that have unprecedented optical, mechanical, electrical, chemical, or biological properties that address needs of human society."

Nowhere else can this revolution have such an immediate payoff as in the area of catalysis. By investing now in new methods for design, synthesis, characterization, and modeling of catalytic materials, and by employing the new tools of nanoscience, we will achieve the ability to design and build catalytic materials atom by atom, molecule by molecule, nanounit by nanounit.

Sources

National Science and Technology Council Committee on Technology (2004). *Nanoscience Research for Energy Needs.* Report of the National Nanotechnology Initiative Grand Challenge Workshop, March 16-18, 2004, sponsored by the National Science and Technology Council Committee on Technology, Subcommittee on Nanoscale Science, Engineering and Technology, and the U.S. Department of Energy Office of Basic Energy Sciences.

National Science Foundation (2003). *Future Directions in Catalysis: Structures That Function at the Nanoscale.* Report of a workshop sponsored by the National Science Foundation, June 19-20, 2003. Workshop Chairs: ME Davis, California Institute of Technology, and TD Tilley, University of California, Berkeley.

U.S. Department of Energy Office of Science (2003). *Basic Research Needs to Assure a Secure Energy Future.* Report of a workshop sponsored by the U.S. Department of Energy Office of Science, Basic Energy Sciences Advisory Committee (BESAC), October 2002. Workshop Chair, John Stringer, Electric Power Research Institute; Co-Chair, Linda Horton, Oak Ridge National Laboratory.

U.S. Department of Energy Office of Science (2002). *Opportunities for Catalysis Science in the 21st Century.* Report of a workshop sponsored by the U.S. Department of Energy Office of Science, Basic Energy Sciences Advisory Committee (BESAC), May 14-16, 2002. Workshop Chair, JM White, University of Texas; Writing Group Chair, J Bercaw, California Institute of Technology.

U.S. Department of Energy Office of Science (2001). "Future Directions of Catalysis Science – Workshop." *Catalysis Letters* 76(3-4):111-124. [Report of a workshop on the Future Directions of Catalysis Science, Berkeley, CA, Feb. 28-March 2, 2001, sponsored by the Chemical Sciences, Geosciences, and Biosciences Division of the U.S. Department of Energy Office of Basic Energy Sciences.]

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