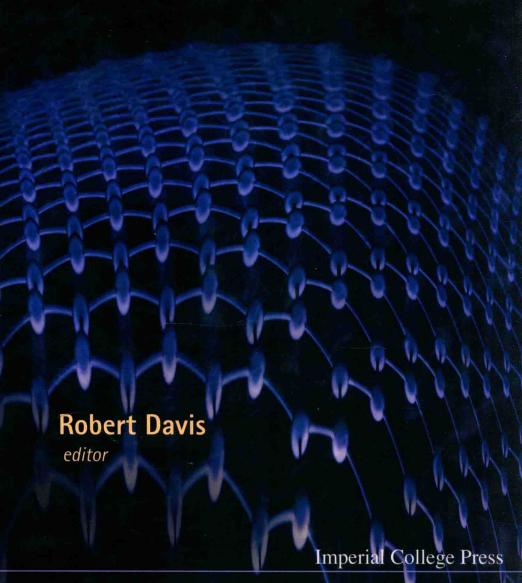
International Assessment of Research and Development in Catalysis by Nanostructured Materials



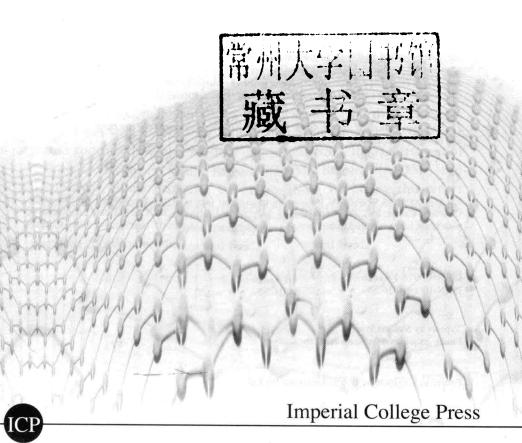
International Assessment of Research and Development in

Catalysis by Nanostructured Materials

Editor

Robert Davis

University of Virginia, USA



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INTERNATIONAL ASSESSMENT OF RESEARCH AND DEVELOPMENT IN CATALYSIS BY NANOSTRUCTURED MATERIALS

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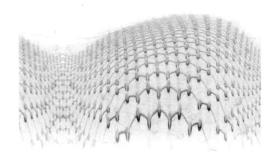
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Dedication

We at WTEC wish to extend our gratitude and appreciation to the panelists for their valuable insights and their dedicated work in conducting this international benchmarking study of R&D in catalysis by nanostructured materials. We wish also to extend our sincere appreciation to the presenters at the North American baseline workshop and to the panel's site visit hosts for so generously and graciously sharing their time, expertise, and facilities with us. For their sponsorship of this important study, our thanks go to the National Science Foundation (NSF), the Department of Energy (DOE), the Air Force Office of Scientific Research (AFOSR), and the Defense Threat Reduction Agency (DTRA). We believe this report provides a valuable overview of ongoing R&D efforts in catalysis by nanostructured materials that can help scientists and policymakers effectively plan and coordinate future efforts in this important field.

R. D. Shelton

Foreword

We have come to know that our ability to survive and grow as a nation to a very large degree depends upon our scientific progress. Moreover, it is not enough simply to keep abreast of the rest of the world in scientific matters. We must maintain our leadership.¹

President Harry Truman spoke those words in 1950, in the aftermath of World War II and in the midst of the Cold War. Indeed, the scientific and engineering leadership of the United States and its allies in the twentieth century played key roles in the successful outcomes of both World War II and the Cold War, sparing the world the twin horrors of fascism and totalitarian communism, and fueling the economic prosperity that followed. Today, as the United States and its allies once again find themselves at war, President Truman's words ring as true as they did a half-century ago. The goal set out in the Truman Administration of maintaining leadership in science has remained the policy of the US Government to this day: Dr. John Marburger, the Director of the Office of Science and Technology Policy

¹ Remarks by the President on May 10, 1950, on the occasion of the signing of the law that created the National Science Foundation. *Public Papers of the Presidents* 120:338.

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(OSTP) in the Executive Office of the President made remarks to that effect during his confirmation hearings in October 2001.²

The United States needs metrics for measuring its success in meeting this goal of maintaining leadership in science and technology. That is one of the reasons why the National Science Foundation (NSF) and many other agencies of the US Government have supported the World Technology Evaluation Center (WTEC) and its predecessor programs for the past 20 years. While other programs have attempted to measure the international competitiveness of US research by comparing funding amounts, publication statistics, or patent activity, WTEC has been the most significant public domain effort in the US Government to use peer review to evaluate the status of US efforts in comparison to those abroad. Since 1983, WTEC has conducted over 60 such assessments in a wide variety of fields, from advanced computing, to nanoscience and technology, to biotechnology.

The results have been extremely useful to NSF and other agencies in evaluating ongoing research programs, and in setting objectives for the future. WTEC studies also have been important in establishing new lines of communication and identifying opportunities for cooperation between US researchers and their colleagues abroad, thus helping to accelerate the progress of science and technology generally within the international community. WTEC is an excellent example of cooperation and coordination among the many agencies of the US Government that are involved in funding research and development: almost every WTEC study has been supported by a coalition of agencies with interests related to the particular subject at hand.

As President Truman said over 50 years ago, our very survival depends upon continued leadership in science and technology. WTEC plays a key role in determining whether the United States is meeting that challenge, and in promoting that leadership.

Michael Reischman
Deputy Assistant Director for Engineering
National Science Foundation

² http://www.ostp.gov./html/01_1012.html.

Abstract

This WTEC panel report assesses the international research and development activities in the field of catalysis by nanostructured materials. Catalysis is important for a wide variety of processes that impact manufacturing, energy conversion, and environmental protection. This study focused specifically on solid catalysts and how nanoscale structures associated with them affect their reactivity. The principal technical areas of the study are (a) design and control of synthetic nanostructures; (b) nanoscale characterization of catalysts in their working state; (c) theory and simulation; and (d) applications. The panel visited over 40 institutions and companies throughout East Asia and Western Europe to explore the active research projects in those institutions, the physical infrastructure used for the projects, the funding schemes that enable the research, and the collaborative interactions among universities, national laboratories, and corporate research centers.

A bibliometric analysis of research in catalysis by nanostructured materials published from 1996 to 2005 was conducted as part of this WTEC study. The total number of published papers as well as the expected total number of citations of those papers revealed a growing focus on this subject. Western Europe was the numerical output leader in the world; US

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output, while published in high-impact journals, was relatively stagnant, and the number of published papers originating from China was growing exponentially and expected to exceed that from the United States in the latter half of this decade. China's rapidly expanding economy together with its growth in large-scale chemical and refining plants motivate its significant commitment to catalysis research.

The panel found that cooperation between universities and companies in catalysis R&D is common in Europe and Asia, presumably because of a more favorable intellectual property environment outside of the United States. In the area of catalyst synthesis, there is substantial activity to develop microporous materials with controlled mesoporosity and to prepare nanosized particles with preferentially exposed crystal planes. Recent advances in spectroscopy and microscopy allow the nanostructures of catalyst particles to be examined under more realistic environmental conditions approaching those of industrial reactions. Electronic structure methods and molecular simulations are now considered to be necessary tools for use alongside experiments to help guide catalysis research. The applications of much of the research observed by the panel are directly related to energy and the environment.

Executive Summary

Robert J. Davis

The science and technology of catalysis are important in the production of modern medicines, new fibers for clothing and construction, a wide variety of consumer products, cleaner-burning fuels, and environmental protection. The US chemical industry, which relies heavily on catalysis, had record exports in 2007 and its first trade surplus since 2001. Furthermore, catalyst technologies account for over US\$1 trillion of revenues in the US economy and about a third of its material GDP. Catalysts are considered the engines that power the world at the nanometer scale and are generally considered to be the most successful application of nanotechnology. For these reasons, the World Technology Evaluation Center initiated a study in 2006 to assess the research and development activities related to catalysis by nanostructured materials under the sponsorship of the National Science Foundation (NSF), the Department of Energy (DOE), the Air Force Office of Scientific Research (AFOSR) and the Defense Threat Reduction Agency (DTRA). The information from the assessment will be used to identify high-impact research areas worth exploring in US R&D programs, clarify research opportunities and needs for promoting progress in the field, identify opportunities and mechanisms for international collaboration, and evaluate the position of foreign

research programs relative to those in the United States. The principal technical focus areas of the study were

- design and control of synthetic catalytic structures
- · nanoscale characterization of catalysts in their working state
- theory and simulation
- applications.

WTEC recruited a panel of eight US experts in the field to perform the assessment. Although a worldwide assessment of this kind normally begins with a benchmarking exercise to establish the state-of-the-art in US R&D programs, a report from the 2003 US National Science Foundation workshop "Future Directions in Catalysis: Structures that Function at the Nanoscale" (NSF, 2003) served as the reference point for US activities in the focus area of the study. Therefore, the current project was performed in the following four phases:

- (1) Conduct a bibliometric analysis to establish world trends in publishing. The analysis examined publication trends by various countries over the last decade. Results were used to confirm and identify new sites selected by the panelists to visit.
- (2) Visit a number of the world's leading university, government, and industry laboratories. The WTEC panelists visited 20 sites in China, Japan, and the Republic of Korea during June of 2007 and 22 sites in Europe in September of 2007.
- (3) Report findings in a public workshop. The panelists reported their findings to the US sponsors, the catalysis community and the general public at a workshop held at the FDIC L. William Seidman Center in Arlington, VA, on November 29, 2007. The workshop, entitled "Assessment of International R&D in Catalysis by Nano-structured Materials", was a public forum in which panelists presented overall findings, specific examples from the site visits, and general conclusions. The workshop also allowed for discussion and critical review of the findings.
- (4) Compile the findings into a written report. This document represents the written record of the study that will be made available to the

sponsors, funding agencies, policymakers, the catalysis community, and the general public. This report is available on the Internet at http://www.wtec.org/catalysis/.

Principal Findings

Bibliometric analysis of catalysis papers

Several important quantitative outputs were determined by the bibliometric analysis (see full analysis in Appendix B). First, catalysis papers in the decade of the study, 1996-2005, represented about 1/60th of the world science output, and the growth rate in catalysis papers (5.4%) exceeded that of all science papers (2.9%), indicating a growing importance of catalysis research in the world. The output of catalysis papers by 13 Western European countries exceeded the total produced by the United States by almost a factor of two. Moreover, there was a significant growth in the number of papers from the People's Republic of China from 1996-2005, while the number of papers from the United States over the same time period was essentially stagnant. In 1996, the catalysis papers from the United States outnumbered those from China by a factor of 6; however, the large disparity between China and the United States was largely eliminated by 2005, and reasonable extrapolation of the exponential growth of Chinese output suggests that the United States now lags China in the number of catalysis papers.

A second quantitative aspect of the bibliometric analysis involved a country's relative commitment (RC) to catalysis. The RC measures the importance of catalysis research within a particular country, with the RC value for the entire world being unity. The very high relative commitment of China (RC > 2) to catalysis research over the decade of the WTEC bibliometric study is consistent with its exponential growth in published papers and contrasts with a very low commitment of the United States to catalysis research (RC \sim 0.6). The relative commitment of Western Europe to catalysis varies by country, but is generally near the world average (RC = 1).

In terms of qualitative comparisons, the papers published by US researchers appear in journals with the highest potential impact, whereas

the papers published in East Asia appear in journals with below average impact factors. The countries of Western Europe publish in journals with impact factors near the world average for the field. Since the Western European countries publish a high volume of papers, the total impact from Western Europe dominated the world over the decade of the WTEC bibliometric study, and the gap between Western Europe and the United States widened over that decade.

The results of the WTEC bibliometric analysis suggest that the United States had a significant, but not dominant, position in catalysis research over the decade 1996–2005. Western Europe led the world in both total number of papers published and the total citation impact. However, the very high relative commitment of East Asia to catalysis research, particularly in China, has fueled an exponential growth in the number of published papers in the last decade and will soon challenge the position of both the United States and Western Europe.

Financial support of catalysis research

The financial models used to support catalysis research vary widely around the world. As a baseline for comparison, the US National Science Foundation and Department of Energy support catalysis research at universities at a level of approximately US\$30 million per year, with nearly half of that originating from the Basic Energy Sciences program at DOE. The Catalysis and Biocatalysis Program at NSF, together with contributions to special programs such as Nanoscale Interdisciplinary Research Teams (NIRT), Nanoscale Exploratory Research (NER), and Partnerships for International Research and Education (PIRE), contribute approximately US\$7 million per year to US university research. The total support from the DOE Office of Science, the DOE Technology Offices, other governmental agencies, and US business for catalysis research at the US national laboratories is estimated to be about US\$45 million. Although catalysis research is also funded by other agencies of the US government such as the Department of Defense and by the private sector through corporate contracts, the major research activities in fundamental catalysis are supported by NSF and DOE.

The different financial models used throughout the world all appear to be effective at supporting catalysis research, and no single system can be declared as the best. However, certain aspects of each deserve close examination for possible adoption in the United States. For example, the sustained level of baseline funding provided to a science-oriented institution such as the Fritz Haber Institute (FHI; see Site Reports-Asia on the International Assessment of Research in Catalysis by Nanostructured Materials website, www.wtec.org/private/catalysis; password required, contact WTEC) allows for effective utilization of a highly trained research staff that is necessary to build the world's next-generation scientific instruments. However, a stable funding stream is not the only unique feature that allows the institution to function at a very high level scientifically. Justification of research directions at the FHI is based on recommendations from an external evaluation committee of scientific experts from around the world instead of on classical numerical outputs such as papers and patents. The stable source of funding for long-term research goals at the FHI contrasts with the typical three-year granting cycle at the US government agencies, which also require yearly justifications for grant expenditures. This difference in funding strategy between the US government and the FHI was highlighted during the WTEC visit as a major reason why certain kinds of research and instrument development are unique to the FHI.

The consortia model developed within and throughout the European countries is another strategy for funding research. These consortia tend to be most effective within a single country, presumably because of the ease of communication, shared cultural identity, and geographic proximity of participating institutions. Although pan-European initiatives have also experienced success, a significant fraction of funding in those initiatives is dedicated to travel and collaboration instead of directly supporting research.

European and Asian countries have done an excellent job combining academic research with national laboratory activities. The combination is almost seamless at many institutions, with principal investigators, professors, doctoral students, and research staff members working together on common goals. There appears to be a more significant separation between academic catalysis research in the United States and its complement at the mission-oriented DOE national laboratories.

Support of doctoral students and postdoctoral researchers on US research grants tends to consume the major fraction of direct charges. In countries like China and Korea, government programs that fund students directly for their graduate education in areas of national importance remove the need to fund students directly on research grants. Although it is unclear whether or not that system is superior to funding students directly on grants, it does appear to be similar to the graduate training grant programs in the United States that are common in other fields.

WTEC panelists found significant industrial collaborations at most of the sites and had the impression that industrial support was more prevalent outside of the United States. The reasons appear to be many, such as a lower cost of performing research outside of the United States, a more cooperative intellectual property environment outside of the United States, and possible access to emerging world markets for the next users of catalytic technologies. Moreover, the panel noted in its visits overseas the high quality of pilot plant facilities and catalytic reactor systems capable of industrial operating conditions located within academic settings. The infrastructure for fundamental research on catalyst synthesis and characterization combined with industrially-relevant catalyst testing appeared to exceed that of typical academic catalysis laboratories in the United States.

Routine equipment for catalysis research such gas chromatographs, reactors, vacuum chambers, adsorption systems, and bench-top spectrometers, as well as major research instruments such as electron microscopes, nuclear magnetic resonance spectrometers, and X-ray diffractometers, are generally available in labs worldwide. In addition, researchers appear to have ready access to synchrotron light sources for advanced *in situ* characterization of catalysts. However, the WTEC panelists reported a significant concern with the aging US catalysis infrastructure—compared to that observed in East Asia and Europe. The difficulties US researchers currently encounter with acquisition of new instruments routinely used for catalysis research could severely impact US competitiveness in the very near future.

General Observations

Catalysis is often associated with large-scale chemical, petrochemical, or oil refinery processes, which are areas of rapid growth in Asia but are fairly

stagnant areas in the United States and the European Union. Although Asia's rapidly expanding economy accounts for its major growth in catalysis research, the reasons for the dominant position of Western Europe in catalysis research output are not so straightforward. Several key factors are likely to contribute to this result. First, catalysis is generally viewed outside of the United States as a fundamental science that enables discovery and development of technology in a variety of energy- and chemicals-related fields. Therefore, catalysis research is pursued in chemistry and physics departments throughout Europe, with much smaller levels of activity in European chemical engineering departments. Within the United States, heterogeneous catalysis has been viewed as a mature field that is studied mainly in chemical engineering departments. Chemistry departments in the United States tend to support much more fundamental studies involving model surfaces in pristine environments, homogeneous or single-site molecular catalysis, and biocatalysis. This artificial division allowed heterogeneous catalysis in the United States to be incorrectly perceived as an applied field of research instead of one with the potential for fundamental discovery.

Another reason European catalysis appears to have a dominant position is the close coupling of universities and national laboratories with industry. Companies within several of the countries the WTEC panel visited appear to campaign for catalysis research at the national level. This kind of advocacy support from companies, together with research contracts involving universities and government labs, indicates a significant role of the private sector in setting research directions.

Moreover, the current intellectual property (IP) environment in Europe appears to foster university-company relations, at least more so than in the United States. However, there are indications that European universities are beginning to explore the position of many US universities on IP ownership and may soon move in the direction of the United States.

Finally, the overall level of investment in catalysis research in Europe simply appears to be higher than that in the United States. Although the United States is starting to see large block grants from companies such as BP and the Dow Chemical for catalysis research at universities, the combined investment of the US government (mainly NSF and DOE) and the industrial sector in university and national laboratory research appears to be far below that of the European countries.

The WTEC panelists observed the use of high-throughput instrumentation in both Asia and Europe. For example, robotic synthesis of zeolite materials and high-throughput reaction testing allowed for discovery of new catalytic materials with unique properties at the Instituto de Tecnología Química (ITQ) in Valencia, Spain (see Site Reports-Europe on the International Assessment of Research in Catalysis by Nanostructured Materials website, www.wtec.org/private/catalysis; password required, contact WTEC). Also, the Center for Microchemical Process Systems at KAIST (Korea Advanced Institute of Science and Technology) makes extensive use of high-throughput screening methods for discovery of new materials. New instrumentation recently purchased at institutions throughout Asia and Europe was aimed at rapid analysis of catalyst samples. Since research abroad is often carried out in major centers of activity, some of the instrumentation was actually invented and constructed inhouse. This model contrasts with the operation of most US academic laboratories, which have neither in-house expertise for tool creation nor the resources for tool construction.

The WTEC panel also noted the effective use of permanent research staff positions in laboratories outside of the United States. In the vast majority of sites visited, including those associated with institutes and universities, the number of dedicated staff members in support of the research activities appeared to far exceed those associated with US laboratories. The employment of highly skilled technical staff members at the Fritz Haber Institute was highlighted during the WTEC visit as a major reason why next-generation research instruments can be designed and built within the facility. The instruments were far too complex to be constructed solely by graduate students and short-term postdoctoral researchers. The US current funding models do not support the same level of technicians, and academic institutions do not appear to have funds available for additional positions; in fact, many US researchers are experiencing a decrease in technical staff at their universities.

Technical Themes of the Study

The chapters in this report present the findings of the panel on the technical themes of the study: synthesis, in situ characterization, theory and