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Catalyst Technology Roadmap Report

N.B. Jackson

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Catalyst Technology Roadmap Report

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ABSTRACT

This report outlines the future technology needs of the Chemical Industry in the area of catalysis and is a continuation of the process that produced the report *Technology Vision 2020: The U.S. Chemical Industry* and the Council for Chemical Research's (CCR) Chemical Synthesis Team follow-up work in chemical synthesis. Vision 2020 developed a 25-year vision for the chemical industry and outlined the challenges to be addressed in order to achieve this vision. This report, which outlines the catalysis technology roadmap, is based on the output of the CCR's Chemical Synthesis Team, plus a workshop held March 20-21, 1997, which included about 50 participants, with catalysis experts from industry, academia, and government. It is clear that all participants view catalysis as a fundamental driver to the economic and environmental viability of the chemical industry. Advances in catalytic science and technology are among the most crucial challenges to achieving the goals of the chemical industry advanced in *Vision 2020*.

EXECUTIVE SUMMARY

This report outlines the future technology needs of the Chemical Industry in the area of Catalysis and is a continuation of the process which produced the report *Technology Vision 2020: The U.S. Chemical Industry* and the Council for Chemical Research's (CCR) Chemical Synthesis Team follow-up work in chemical synthesis. *Vision 2020* developed a 25-year vision for the chemical industry and outlined the challenges to be addressed in order to achieve this vision. This Catalysis Technology Roadmap is based on the output of the CCR's Chemical Synthesis Team plus a workshop held March 20-21, 1997, that included about 50 participants, with catalysis experts from industry, academia, and government.

The two major goals which emerged from both the CCR Chemical Synthesis Team and the workshop were 1) acceleration of the catalyst development process and 2) development of catalysts with selectivity approaching 100%. Acceleration of catalyst development will have a significant economic effect and will contribute to the leadership of the US chemical industry. The workshop identified and ranked the areas of application of catalyst technology in which improvements of catalytic processes would have a significant impact on meeting the goals of *Vision 2020*. Discontinuities in technology development in these areas could have an enormous economic and environmental impact. These categories are, in order of importance as defined by the workshop, selective oxidation, hydrocarbon activation, byproduct and waste minimization, stereoselective synthesis, functional olefin polymerization, alkylation, living polymerization, and alternative renewable feedstocks. Both the CCR Chemical Synthesis Team and the workshop identified and discussed the critical needs within catalysis. The workshop discussed and ranked these needs. The four primary needs that were identified are listed below.

1. Enable catalyst design through combined experimental and mechanistic understanding, and improved computational chemistry.
2. Development of techniques for high throughput synthesis of catalysts and clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation.
3. Better in situ techniques for catalyst characterization
4. Synthesis of catalysts with specific site architecture

Research investments for meeting these critical needs were recommended by the workshop participants. The potential research investments were classified into short (3-5 years), medium (5-9 years) and long (>9 years) term research endeavors. The details of those investments are in the report.

It is clear from both the active participation of many chemical industry representatives in the CCR Chemical Synthesis Team and the Workshop, as well as the discussions at the Workshop, that all participants view catalysis as a fundamental driver to the economic and environmental viability of the chemical industry. Advances in catalytic science and technology are among the most crucial challenges to achieving the chemical industry goals advanced in *Vision 2020*.

ACKNOWLEDGEMENTS

The Catalyst Technology Roadmapping Workshop was sponsored by the Council for Chemical Research and the DOE Office of Industrial Technology. The workshop was organized by Nancy Jackson, Sandia National Laboratory, and Tom Baker, Los Alamos National Laboratory. The lodging, conference room, and meal logistics were organized by David Schutt and Diane Ruddy, American Chemical Society. The report was compiled by Nancy Jackson. The workshop facilitator was Arnold Baker, Sandia National Laboratory, and the panel discussions were facilitated by Jerry Ebner, Monsanto, Kevin Ott, Los Alamos National Laboratory, Tom Baker and Nancy Jackson. Reporters for the panel discussions were Mark McDonald, Federal Energy Technology Center, Kevin Burgess, Texas A&M University, Steven Rice, Sandia National Laboratory, and Rosemarie Szostak, Clark Atlanta University.

CATALYST TECHNOLOGY ROADMAP

BACKGROUND

This report outlines the future technology needs of the Chemical Industry in the area of Catalysis and is a continuation of the process which produced the report *Technology Vision 2020: The U.S. Chemical Industry*. *Vision 2020* developed a 25-year vision for the chemical industry and outlined the challenges to be addressed in order to achieve this vision. This report was a joint project of the American Chemical Society (ACS), The Chemical Manufacturers Association, the American Institute of Chemical Engineers, the Council for Chemical Research (CCR), and the Synthetic Organic Chemical Manufacturers Association. Four technical disciplines were identified as being required for fulfilling this vision, of which one was “new chemical science and engineering technology”. The report recognized that chemical science development is the most fundamental driver of advances within the chemical industry and the most crucial aspect for maintaining and improving the competitiveness of the US chemical industry. Chemical synthesis was recognized as one of three primary areas within the chemical sciences that requires long term investment in R&D. Chemical synthesis was defined to include inorganic and organic synthesis (turning raw materials into useful chemicals and products) by either catalytic or non-catalytic processes. However, catalysis-based chemical synthesis accounts for 60 percent of today’s chemical products and 90 percent of current chemical processes. Catalysis development and understanding is essential for the majority of chemical synthesis advances. Because the topic of chemical synthesis is so broad and the topic of catalysis is so crucial to chemical synthesis, catalysis was chosen be roadmapped individually.

A Chemical Synthesis Team was formed under the auspices of the CCR and this team identified cross cutting needs and targets that were applicable to all catalyst systems at their December 6, 1996 meeting. Participants in the CCR Chemical Synthesis Team are listed in Appendix A. The CCR Chemical Synthesis Team also identified a list of critical needs in the area of catalysis. To further the catalysis roadmapping effort, a workshop was held March 20-21, 1997, at the ACS Headquarters which included 48 participants from industry, academia, and government. The workshop goal was to prioritize the critical research needs of the U.S. chemical industry and their accompanying research investments. Participants and agenda are in Appendix B. A brief discussion of the methodology used at the workshop is described in Appendix C. In addition to the workshop, a questionnaire was sent to a cross-section of the chemical industry (diversified manufacturers, oil companies, specialty chemical outfits, catalyst manufacturers, and pharmaceutical houses) prior to the workshop to obtain a broader based starting point for the discussion. A copy of the questionnaire

and the tabulated results are in Appendix D. These results were reported to the participants at the beginning of the workshop.

VISION

Since this Catalysis Roadmap is being drawn under the umbrella of the *Vision 2020* process, it should be noted that the roadmap was conceived with the understanding that we were trying to achieve the vision laid out in *Vision 2020* and our portion of it was Catalysis. In the end, all aspects of this Catalysis Roadmap are aimed towards fulfilling the vision statements in *Vision 2020*. This vision includes maintaining the vitality and world leadership of the US chemical industry while maintaining high standards of safety and promoting sustainable development.

CRITICAL REQUIREMENTS/GOALS FOR CATALYSIS IN THE NEXT 25 YEARS

Catalysis is a broad technical field and not, in and of itself, a product. It was the consensus of the workshop that the field of catalysis is different than say, the automotive industry, which can set a quantitative target of, for example, developing an energy efficient vehicle that gets 80 mpg by the year 2005. Similar targets could be set for individual processes/catalysts, but the chemical industry is so large that to target just one catalyst/process would have little impact on overall industry energy usage or waste minimization. It was thought that more general advancements within the field of catalysis could have profound economic, environmental, and energy usage impacts within the industry.

The two major goals which emerged from both the CCR Chemical Synthesis Team and the workshop were 1) acceleration of the catalyst development process and 2) development of catalysts with selectivity approaching 100%. Acceleration of catalyst development will have a significant economic effect and will contribute to the leadership of the US chemical industry. In order to accelerate development the CCR Chemical Synthesis Team noted that several cross-cutting technologies would need to be developed.

- 1) High throughput/diversity catalyst synthesis and screening
- 2) Faster characterization systems
- 3) Rational catalyst design which uses computation-computer techniques both empirical and fundamental
- 4) Better fundamental understanding of intermediate pathways, transition states and in situ monitoring

The development of catalysts with selectivity approaching 100% is a need driven by economics and waste minimization considerations and the technologies needed are the same four as listed above.

The participants first identified and ranked the areas of application of catalyst technology in which improvements of catalytic processes would have a significant impact on meeting the goals of *Vision 2020*. Discontinuities in technology development in these areas could have an enormous economic and environmental impact. These categories are listed in Table 1 and Figure 1. During the discussion on these categories, workshop participants noted that all these processes require low temperature, high selectivity routes, indicating success in these areas would lower energy requirements for many large processes. Green catalytic systems were also considered, but the general consensus of the workshop was that this area is implicit in *Vision 2020*. Alkylation chemistry was chosen since it is a process, rather than solid acid/base catalysis, which was originally suggested. Controlling catalyst stability or lifetime was also not seen as an individual area, but is implicit within any endeavor in catalysis. Reactor engineering was seen as critical, and some thought integral, to catalysis, but the consensus of the group was to leave that topic to another workshop.

Table 1. Areas of application of catalyst technology in which improvement of catalytic processes would make significant progress toward meeting the goals of *Vision 2020*

CATALYST TECHNOLOGY	INDUSTRY*	ALL
Selective oxidation	27	23
Alkane activation	21	21
Byproduct and waste minimization	13	15
Stereoselective synthesis	9	9
Functional olefin polymerization	8	9
Alkylation	8	10
Living polymerization	6	6
Alternative feedstocks and renewables	4	7

*Process of ranking is described in Appendix C.

RANKING CRITERIA

DECIDING THE CRITERIA FOR RANKING THE MOST CRITICAL NEEDS IN ADVANCING CATALYSIS

Before the critical needs were ranked, the participants discussed and prioritized the criteria to be used in ranking the critical needs. A straw man list of criteria was introduced and each suggested criterion was discussed. The ranking criteria are listed in Table 2.

Table 2. Straw man criteria for ranking research investments

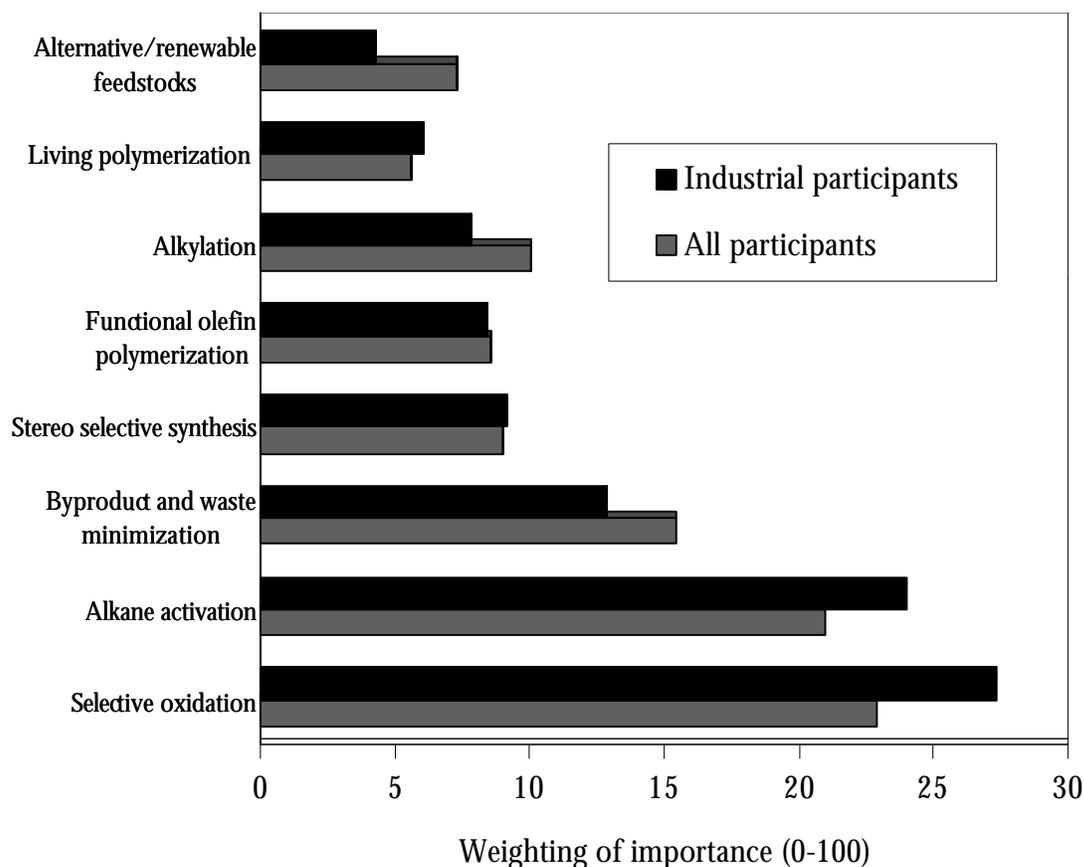
Impact of technology advances
Timeliness of the impact of technology advances
Probability of successful technology development
Cost of investment relative to the potential benefit of the technological advance

Appropriateness of a government role in developing associated advanced technologies

Regarding impact of technological advances, the participants discussed whether “impact” had to mean that the advance directly affected a process or whether it would affect catalysis research. The general consensus of the workshop was that “impact” meant an impact to a wide range of processes and that the impact must affect the yield and simplicity (number of unit operations) of the process. The CCR Chemical Synthesis Team defined impact as being related to a nonincremental improvement that would move the industry to a new level. Impact leads to big steps and big discontinuities. The workshop participants recognized that government perceives impact as the effect on society: lowered energy use, waste minimization, etc.

There was a discussion about the next four criteria and their inter-relatedness. There were comments that if there was a high probability of success, then perhaps industry should be developing that technology. Although it is important to work on good ideas, it is important not to limit research to ideas that have a high probability of success. Big discoveries have often come from accidental discoveries, which indicates the importance of supporting catalysis research in general. Most agreed that they were willing to take big risks for big impact technologies. Broad, across-the-industry relevance is important and some thought cost should not be significant. In fact, there was discussion about removing that criteria from the list. However, the consensus was that cost is an issue for funding agencies, so realistically, it needs

Figure 1. High impact areas within catalysis ranked by all participants and industrial participants



to be included. A question about how “benefit” should be defined was answered by the participants to mean relevance to *Vision 2020* and applicability across the chemical industry. The general consensus was that government should fund high risk research and that the probability of the successful *technology* development is not important but the probability of good science is a better criteria. There was a general sense that probability of success is important but probability of commercial development is not as important. Another criteria that was suggested was the willingness of industry to work together as a group to solve the problem. Concern was expressed about the ability of catalysis to attract the best and brightest of students to the field, however, many thought this concern should be addressed in another forum. Discussion of the appropriateness of the government role led to a consensus that the government should fund research that industry is not willing to do on its own, i.e. long term basic research and precompetitive research rather than work on specific products and processes. Therefore the participants suggested changing the ranking criteria to reflect these concerns. The workshop list of ranking criteria and the importance of those criteria are listed in Table 3.

Table 3. Ranking criteria in order of importance

	INDUSTRY	ALL PARTICIPANTS
Impact of research on technology	45	40
Timeliness of research	17	15
Probability of technical success	14	15
Cost of investment relative to the potential benefit	14	14
Precompetitive research stage	9	14

CRITICAL NEEDS FOR ADVANCING CATALYSIS

The CCR Chemical Synthesis Team developed a list of critical needs for advancing the state of catalysis technology. These are listed in Table 4 and were used as the starting point for discussion in the workshop.

The first two needs listed in Table 4 address the desire to make more efficient libraries of hetero/homogeneous catalysts for accelerated empirical screening and to develop combinatorial methodologies for catalysis.

The interesting point about the workshop discussion on the third critical need, better in situ techniques for catalyst characterizations, is that there was virtually no discussion on this topic and it was unanimously agreed to as a critical need.

A CCR Chemical Synthesis Team member asked at the workshop that the word “rational” be removed from the fourth critical need statement. The participants of the workshop wanted to make it clear that an experimental component is necessary for mechanistic understanding and suggested a word change to reflect that point.

A participant at the workshop pointed out that the technique of supporting a homogeneous catalysts on a solid support may never work and that what was really important could be phrased differently. A broader definition was agreed upon: “Develop innovative synthesis techniques to prepare single site catalysts.”

Table 4. Critical Needs in Catalysis (not ranked)

CRITICAL NEEDS DEVELOPED BY THE CCR CHEMICAL SYNTHESIS TEAM, DECEMBER 6, 1996
--

1. Simple techniques for rapid throughput catalyst synthesis with a focus on molecular diversity, i.e. a wide range of catalyst compositions
2. Clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation
3. Better in situ techniques for catalyst characterization
4. Enable rational catalyst design through combined mechanistic understanding and improved computational chemistry
5. Development of techniques to prepare supported homogeneous catalysts
6. Exploitation of interfaces of chemical synthesis with biotechnology and material science
7. Development of multi-step, "one pot" reactions
8. Identification of new approaches to big stake areas such as selective oxidation, solid acid/base catalysis, living polymerizations, functional olefin polymerization

Critical need #6 was identified as an approach rather than a need and although there were examples where overlap with these fields were important (ability to build nano-level materials such as material scientists strive towards; enzyme mimics as catalysts are an example of overlap with biotechnology), it was agreed that this critical need should be dropped.

There was discussion about the seventh critical need since it was not clear to everyone what it meant. To clarify this need, it was agreed to be restated as "Development of multifunctional catalysts for carrying out multistep reactions."

The eighth critical need was thought by some to be an application and not a method. As a consequence, this critical need was removed and the high impact processes mentioned in the eighth critical need were expanded upon and ranked. These data are shown in Table 1.

During the course of the discussion, six new critical needs were suggested:

- 1) Novel catalytic reactor designs
- 2) Controlling catalyst stability
- 3) Attract best and brightest minds to catalysis
- 4) Innovative approaches to catalysis using non-toxic reagents and with minimum production of by-products

This suggestion was particularly controversial to some industrial workshop participants because of the call for non-toxic reagents. Minimum production of by-products was uniformly attractive to industry participants because it implies a lower cost process. There was a suggestion to re-state this critical need to "Development of green catalyst systems." This would also include catalysts for recycling.

- 5) Nanoscale control of catalyst site architecture, for example, learn to develop a catalyst with one particular surface orientation
- 6) Reduce barriers to collaboration between institutions, public and private

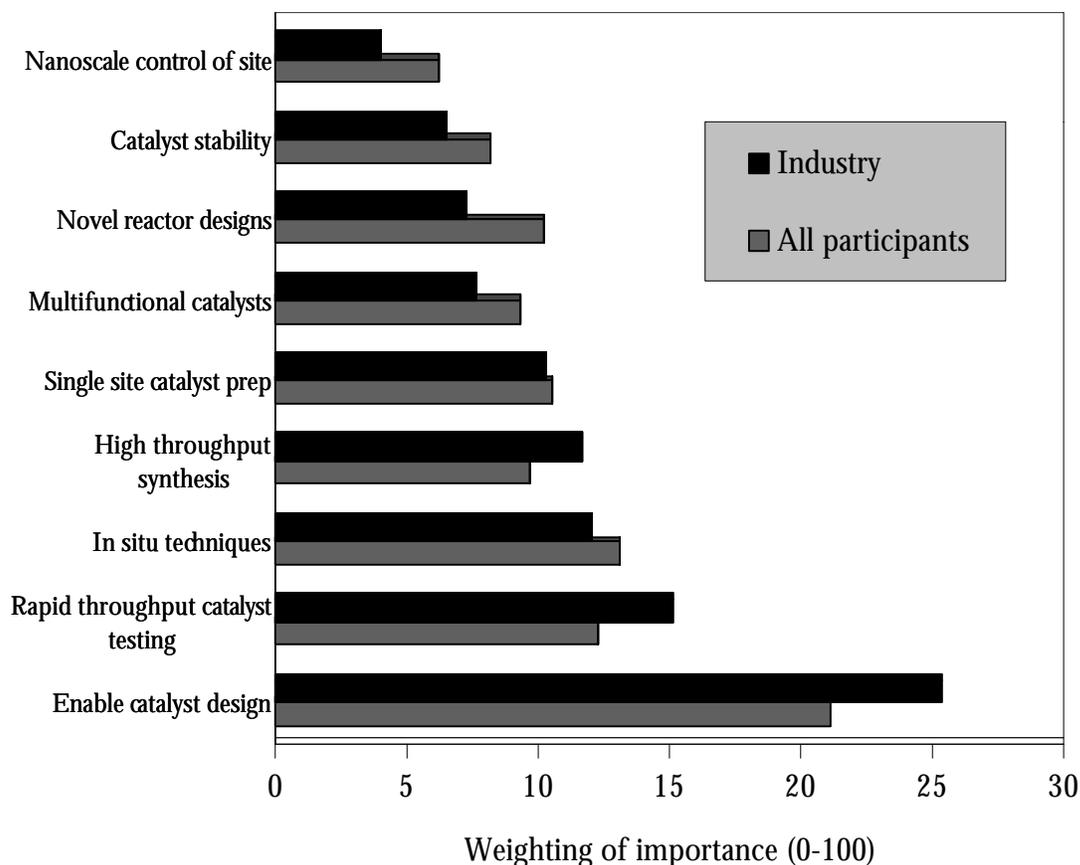
Table 5. Critical Needs in Catalysis ranked in order of priority

RANK	CRITICAL NEED
1	Enable catalyst design through combined experimental, mechanistic understanding, and improved computational chemistry
2	Clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation
3	Better in situ techniques for catalyst characterization
4	High throughput synthesis of catalysts
5	Develop innovative synthesis techniques to prepare single site catalysts
6	Development of multifunctional catalysts for carrying out multistep reactions.
7	Novel catalytic reactor designs
8	Controlling catalyst stability
9	Nanoscale control of catalyst site architecture, for example learn to develop a catalyst with one particular surface orientation

The workshop participants thought that reducing barriers to collaborations (6) and attracting the best and brightest (3) were important, but that they were overriding issues affecting all aspects of *Vision 2020*. In addition, the participants thought that green chemistry (4) was a strategic goal, and not a critical need and it was removed from the list.

The final list and ranking that the workshop participants gave the critical needs may be seen in Table 5 and Figure 2.

Figure 2. Ranking of Critical Needs by All Workshops Participants and by Industrial Workshop Participants



RESEARCH INVESTMENTS REQUIRED TO MEET CRITICAL NEEDS

In preparation for identifying and ranking research investments to meet the critical needs, participants agreed to bundle several of the critical needs. Rapid throughput synthesis (#4) and testing (#2) were considered together, and #5, 6, 8, and 9 were merged and redefined as Synthesis of Catalysts with Specific Site Architecture. Eight of the critical needs were thus combined into four categories. Workshop participants split into four groups and identified research investments that were necessary to meet the critical needs. Next they ranked the research investments using the criteria discussed above and given in Table 2 for the critical needs and identified whether the

investments needed were short term, S, (3-5 years), mid-length, M, (6-9 years) or long term, L, (>9 years).

1. Enable catalyst design through combined experimental, mechanistic understanding, and improved computational chemistry.

Areas of research required for meeting this critical need are outlined below. The subheadings under each major topic are not necessarily independent of each other. For example, development of improved computational chemical models may involve methods that are both more realistic and more accurate, and experimental work could incorporate both fundamental mechanistic studies and in situ characterization. Since only a small panel (9 people) was responsible for identifying the subheadings, the panel thought that the lists should not be considered exhaustive. At the workshop, some discussion among the panel members was given to whether development of better computation or code was a useful priority. The general opinion seemed to be that improvements in computation or coding were means to an end rather than an end in themselves. Listed below in order of ranking are the research investments recommended by the panel along with the length of investment required for each area. Figure 3 gives a breakdown of the ranking.

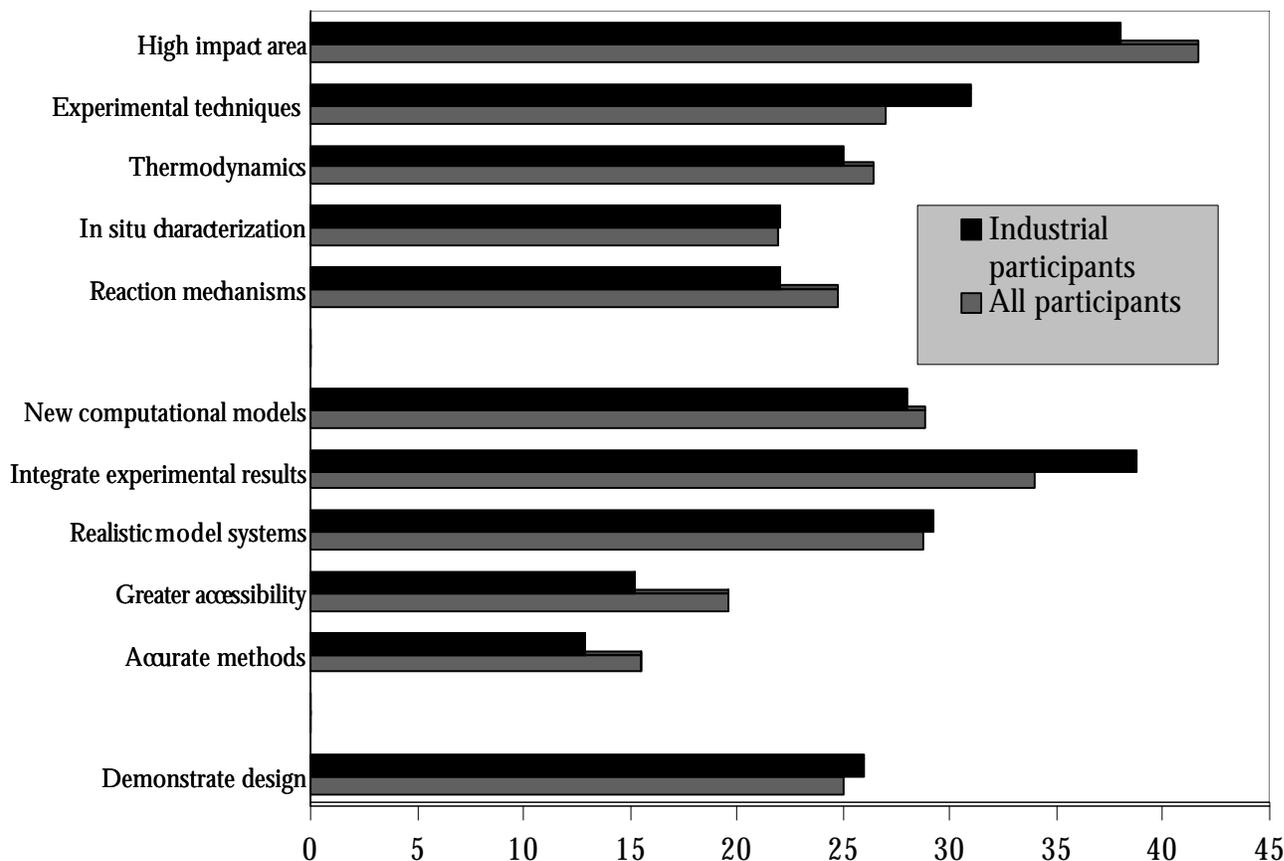
CONDUCT EXPERIMENTS DIRECTED TOWARDS HIGH IMPACT AREAS, ESPECIALLY THE FOLLOWING TYPE OF STUDIES - S,M,L

- Thermodynamic measurements including adsorption and desorption studies, surface reaction studies, and transient species - S, M
- Fundamental reaction mechanistic and kinetic studies - S, M
- In situ characterization studies - M, L
- Development of new and improved techniques with greater temporal, spatial, and species resolution - S, M, L

DEVELOP NEW OR IMPROVED COMPUTATIONAL CHEMISTRY MODELS WITH EMPHASIS ON THE FOLLOWING - S, M, L

- More realistic model systems incorporating complexities of real catalysts such as medium effects and realistic cluster sizes - M, L
- More accurate methods - L
- Methods with greater accessibility for the broader scientific community - S, M
- Methods that better integrate with experimental results in areas such as thermochemistry, kinetics, transport properties, and phase - M

Figure 3. Design of catalysts using computation and experimental information



Development of new or improved experimental techniques was originally considered a topic important enough to be a separate item. A strong majority of the panel chose to make it a sub-heading in the section on experimental work, even though they thought that technique development obviously drives many advancements in experimentation and should not be ignored.

DEMONSTRATE CATALYST DESIGN FROM THE COMBINATION OF EXPERIMENTAL, COMPUTATIONAL, AND MECHANISTIC KNOWLEDGE - S, M, L

The panel was particularly interested in pointing out that very little support has typically been provided for actual catalyst design based on fundamental experimental and theoretical results, but that such an approach is possible today. Given the incremental nature of such science and technology, the lack of funding for catalyst design is not surprising, but given the strong support by

the workshop for catalyst design, the panel felt strongly that actual attempts in this area merit funding.

The panel on catalyst design had 9 members: 5 industrial, 2 academic, and 2 national laboratory, participants.

2. Development of techniques for high throughput synthesis of catalysts and clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation.

Rapid throughput techniques must be developed to enhance the discovery of catalysts for novel reactions or of new catalysts for known reactions. Seven points were outlined for further study and they are listed below in order of importance as ranked by the panel. Details of ranking results may be seen in Figure 4.

MICRO- AND NANO-SCALE ENGINEERING - M, L

This is particularly needed for heterogeneous catalyst systems. Small vessels are required that would enable arrays of catalysts to be developed and encapsulated with the products they generate (gaseous materials).

NEW APPROACHES FOR RAPID DETECTION OF LOW CONCENTRATION OF PRODUCTS - S, M

Assays are required for both homo- and heterogeneous catalysis that would enable rapid detection of products. Leads could perhaps be drawn from bio-assays wherein such tools as fluorescence, radiolabeling, UV-VIS, precipitation, and antibodies are routinely employed.

SYSTEMS FOR PARALLEL SCREENING OF LIBRARIES, PARTICULARLY UNDER DIFFICULT CONDITIONS INCLUDING HIGH TEMPERATURES AND PRESSURES, STRICTLY ANAEROBIC ENVIRONMENTS - M, L

Screening for some reaction types is hard due to constraints imposed by the reaction itself. Techniques are required to overcome this.

NEW CHEMISTRY FOR SYNTHESSES OF LIGAND LIBRARIES - S, M

High throughput screens of catalysis, particularly homogeneous stereoselective catalysts, require that equivalent numbers of ligands are generated. Several techniques can be imagined for doing this, several of which feature solid phase syntheses.

SYNTHESIS OF CATALYST ARRAYS WITH HIGH SPATIAL RESOLUTION - S, M, L

Generation of “catalysts on chips” requires deposition techniques that will enable efficient synthesis of closely packed catalyst arrays.

RAPID TECHNIQUES FOR DETAILED CHARACTERIZATION OF HETEROGENEOUS CATALYST LIBRARIES - M, L

Characterization of catalysts in arrays will be important to correlate overall reactivities with composition.

AUTOMATION FOR RAPID PERFORMANCE TESTING - M

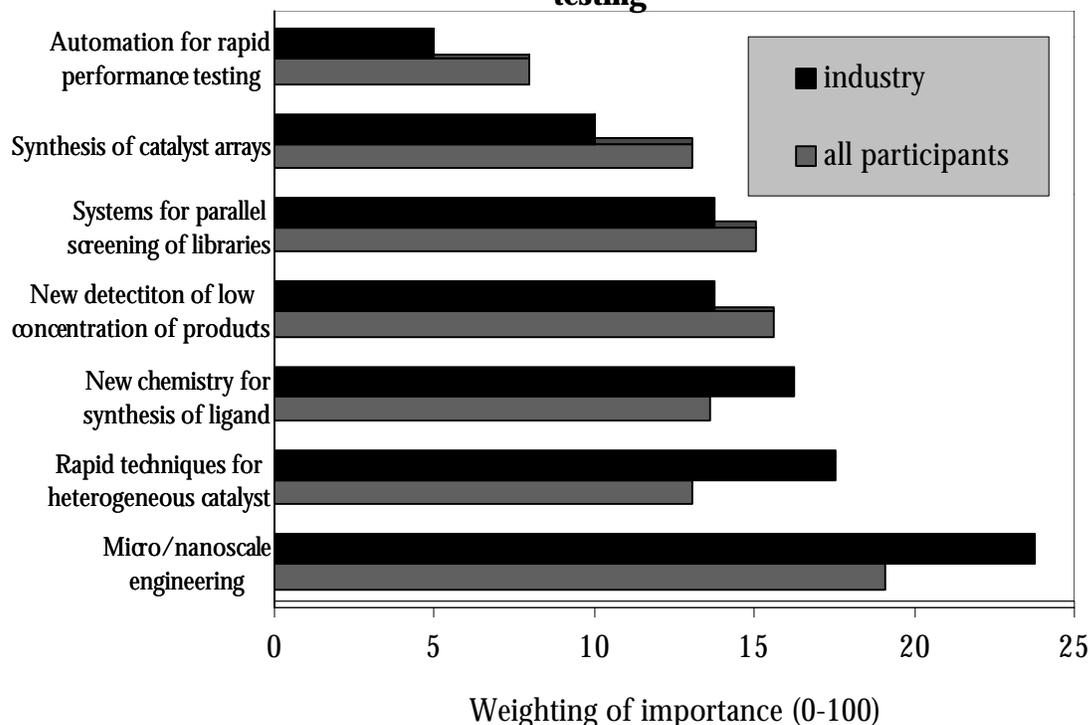
Robotic systems will be required to realize many of the goals outlined in the other sections.

The panel for techniques for rapid synthesis and testing had 11 members: 5 industrial, 4 academics, and 2 national laboratory participants.

3. Better in situ techniques for catalyst characterization

The workshop panel exploring this critical need classified in situ characterization techniques into two broad categories: those which give information on catalyst characteristics and those which give information on reaction characteristics. It was noted that few techniques covered both, such as providing a molecular description of the site and reactive intermediates with temporal resolution under realistic conditions. This includes understanding variables such as structure vs. time; composition vs. time; accessibility of techniques with wide utility; species sensitivity; and spatial resolution. Both improvements of present techniques as well as development of new methods were considered by the workshop panel. The recommended research investments are listed below in ranking order with details shown in Figure 5.

Figure 4. Development of techniques for high through put synthesis and testing



DEVELOPMENT OF X-RAY SPECTROSCOPIES (INCLUDING ABSORPTION) AND X-RAY MICROSCOPY WITH HIGHER SPATIAL, TEMPORAL, AND ENERGY RESOLUTION - M

THREE-DIMENSIONAL TECHNIQUES (PET, MAGNETIC RESONANCE IMAGING, AND NMR SPECTROSCOPY) - M

SCANNING PROBES OR MOLECULAR REPORTERS SUCH AS RADIOTRACERS - L

IN SITU DIFFRACTION AND MICRO-DIFFRACTION TECHNIQUES - S

DEVELOPMENT OF TECHNIQUES FOR NONPLANAR AND ROUGH MATERIALS - M

TECHNIQUES FOR NANO/MESOSCALE TRANSPORT MEASUREMENT FOR MODEL VERIFICATION - M

TRANSIENT TECHNIQUES FOR MEASUREMENT OF PHYSICAL (E.G. THERMODYNAMIC) PROPERTIES, AND THEIR EVOLUTION IN SITU - S

The panel for in situ characterization had 10 members: 2 industrial, 2 academics, 5 national laboratory, and 1 government funding agency participant. 4. *Synthesis of catalysts with specific site architecture*

This is a combination of four critical needs: Develop innovative synthesis techniques to prepare single site catalysts; nanoscale control of catalyst site architecture, development of multifunctional catalysts for carrying out multistep reactions, and controlling catalyst stability. The recommended research investments are listed below in ranking order with details shown in Figure 6.

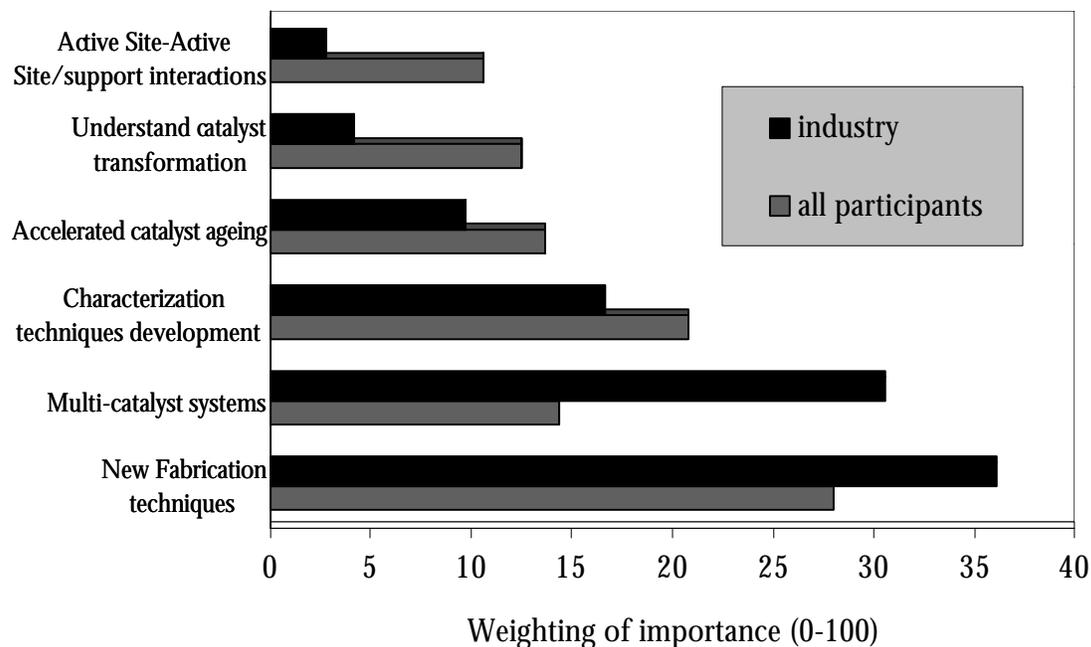
Figure 5. Better in situ techniques for catalyst characterization



NEW FABRICATION METHODS FOR CATALYSTS - S, M, L

The workshop panel that discussed this topic thought that new fabrication/synthesis methods are needed to produce improved catalysts containing highly uniform active sites, either single or multiple sites on an individual catalyst, defined clusters, specific arrays, uniform crystal faces, key metallocenes, and/or controlled pore size materials. Control over the uniformity of active sites is the key to achieving 100 percent selectivity in a given reaction (no waste or by-products). With new constraints continuing to be placed on the industry as a result of increased regulation and the need for better environmental performance, catalyst formulation and synthesis will be a critical function in meeting the needs of the chemical industry.

Figure 6. Synthesis of catalysts with specific site architecture



TECHNOLOGY DEVELOPMENT TO DESCRIBE/CHARACTERIZE SOLID ACTIVE SITE AT ATOMIC LEVEL - M, L

With improved synthesis methods comes the need for development of characterization techniques to more precisely describe the active sites at the atomic level. The tools required for analysis are expected to be diverse and may ultimately hinge on breakthroughs in other unrelated technology areas.

UNDERSTAND/SYNTHESIZE MULTI-CATALYST SYSTEMS - S,M

TECHNOLOGY TO ACCELERATE AGING MEASUREMENTS - L

DESCRIBE CHEMICAL TRANSFORMATION OR THE WAY A CATALYST PHASE ASSEMBLES (E.G., SOL TO CRYSTAL FORMATION) - M, L

UNDERSTAND ACTIVE SITE-ACTIVE SITE AND ACTIVE SITE-SUPPORT INTERACTIONS - M, L

The panel on active site architecture had 11 members: 3 industrial, 3 academic, 4 national laboratory, and 1 federal funding agency participant.

SUMMARY

The two major goals for the chemical industry regarding catalysis were defined as 1) acceleration of the catalyst development process and 2) development of catalysts with selectivity approaching 100 percent. The consensus of the workshop participants was that the most important research investments are those that have the potential to make the greatest impact. It is acceptable for the research to be high risk, long term or costly, but the potential of producing a discontinuity, a big step forward for the chemical industry is important. The workshop also reiterated the sentiment of the industrial questionnaire response regarding the appropriateness of government funding for precompetitive work. The science/technologies that were identified as being most crucial to the field of catalysis included:

- Make design of catalysts possible through a combination of experiment, mechanistic understanding of reactions, and improved computational chemistry
- Develop techniques for high throughput synthesis and testing of catalysts
- Develop better in situ techniques for catalyst characterization
- Develop methods of synthesis of catalysts with specific site architecture

The workshop made suggestions as to where research would be most effectively invested to achieve the above technologies and classified the potential research investments into short (3-5 years), medium (5-9 years) and long (>9) term research endeavors.

The three most important areas of application of catalyst technology in which improvement of catalytic processes would make the most significant progress towards meeting the goals of *Vision 2020* include

- Selective oxidation
- Alkane activation
- Byproduct and waste minimization

It was clear from both the active participation of many chemical industry representatives in the CCR Chemical Synthesis Team and the Workshop as well as the discussions at the Workshop that all participants view catalysis as a fundamental driver to the economic and environmental viability of the chemical industry. Advances in catalytic science and technology are among the most crucial challenges to achieving the chemical industry goals advanced in *Vision 2020*.

APPENDIX A

COUNCIL FOR CHEMICAL RESEARCH CHEMICAL SYNTHESIS TEAM

**Council for Chemical Research
Chemical Synthesis Team**

- Attendance at December 6, 1996 Meeting, Wilmington, DE

Victoria Haynes, Chair
BF Goodrich

Paul Nicholas
BF Goodrich

Brian Goodall
BF Goodrich

Tom Baker
Los Alamos National Laboratory

Alexis Bell
University of California, Berkeley

William Dowd
Dow Chemical Company

Jerry Ebner
Monsanto

Bruce Smart
Du Pont

Harold Myron
Argonne National Laboratory

- Others who contribute(d) to Team's work
George Whitesides
Harvard University

Leo Manzer
DuPont

Matt Tirrell
University of Minnesota

APPENDIX B

WORKSHOP AGENDA LIST OF PARTICIPANTS

AGENDA

CATALYSIS WORKSHOP

*American Chemical Society
1155 16th Street, NW
Washington, DC*

March 20, 1997

Day 1

Continental Breakfast		8:00 AM
Welcome	Nancy Jackson	8:25 AM
OIT Representative	Denise Swink, Dep. Asst. Sec., OIT	8:30 AM
Report on Council for Chemical Research, Committee on Chemical Synthesis	Jerry Ebner Monsanto	9:00 AM
Process Overview/Goals	Dr. Arnold Baker, Facilitator	9:20 AM
Break		9:50 AM
Criteria for Ranking Critical Needs		10:00 AM
Lunch (brought in)		11:30 AM
Critical needs and ranking critical needs	12:30 PM	
Break		2:30 PM
Criteria for ranking research investments	2:45 PM	
Meeting announcements	Nancy Jackson	4:15 PM
Adjourn for day (except for breakout facilitators and reporters)		4:30 PM
Day 2 breakout session facilitator and reporters meeting		4:30 PM

AGENDA

CATALYSIS WORKSHOP

*American Chemical Society
1155 16th Street, NW
Washington, DC*

March 21, 1997

Day 2

Continental Breakfast		8:00 AM
Process overview/goals for Day 2	Dr. Arnold Baker	8:30 AM
Transition into 4 breakout groups		8:45 AM
Identify and rank research investments		9:00 AM
Working lunch		11:30 AM
Breakout group summaries given by reporters		12:00 PM
Wrap up	Nancy Jackson	1:00 PM
Adjourn		1:30 PM

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MARCH 20-21, 1997

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APPENDIX C

RANKING/VOTING PROCEDURE AT WORKSHOP

VITAL ISSUES PROCESS

Workshop Ranking Process

The ranking process at the workshop was conducted by using a written (but not secret) ballot. If, for example, nine items were to be ranked, then each participant was asked to indicate how they would divide \$900 worth of funding among the items. This value was tabulated and averaged for both industrial participants and for all participants. The values included in the report are based on a 0-100 scale for uniformity.

The Vital Issues Process

The Vital Issues Process is a strategic planning tool developed at Sandia National Laboratories. It identifies a portfolio of programmatic activities (an 'investment portfolio') for an organization, aimed at satisfying its high-level goals and objectives. The process requires a high level of stakeholder involvement, thus predisposing acceptance of the programmatic endeavors by those stakeholder communities.

Description

The Vital Issues Process is a multi-stage process, involving a series of day-long, intensive workshops, each of which builds on the results of the previous. The first workshop focuses on definitions, identifying target goals, objectives, (in this case, the vision statements in *Technology Vision 2020*) and/or critical needs describing the type of issues or problems addressed by the sponsoring organization (in this case, the critical needs in catalysis identified by the Council for Chemical Research Chemical Synthesis team), and identifying criteria for issue or problem selection. The next workshop (i.e., the workshop set for March 20-21) uses the selection criteria and the definition of the desired issue or problem to identify and rank a set of such issues. The following workshop (or set of workshops) selects one or more of those identified issues (probably, but not necessarily the highest ranked) and identifies and ranks associated programmatic activities, such as research investments (or Day 2 of our workshop). Subsequent workshops can focus on tasks associated with specific programmatic activities. The outcome of this process can provide key elements for a strategic investment plan or road map. The process is illustrated in Figure C1.

Figure C1

The panel of participants in each workshop may differ, according to the expertise required for the topic at hand. Institutional perspectives which are key to organizational success (such as private sector, state/federal government, and academe) should be identified *a priori* and represented on each panel. Each panel also should reflect a broad range of stakeholder communities. Individual panelists should be selected for their expertise and credibility within their professional communities.

The Vital Issues Process incorporates two primary approaches: a qualitative, or transactional method, which takes a synthesis approach; and a quantitative, or net benefit maximization method, which performs some analysis activities. The transactional method involves dialogue among individuals or groups with some stake in the sponsoring organization's activities. Such dialogue usually focuses on problem or issue definition (which can include definition of an organization's goals and objectives) and criteria for measuring success through problem solution or goal achievement. Participation in the construction, or synthesis, of those definitions allows participants to become invested in the process. The definitions constructed by these synthetic activities form the environment within which a set of alternatives (such as issues or programs) can be identified. Net benefit maximization uses quantitative methods to perform a cost/benefit analysis on a set of given alternatives, seeking to identify the alternative that provides the greatest social (or organizational) good according to some set of criteria.

Both methods are applied in each workshop of the Vital Issues Process. The agenda leads off with a discussion of the topical area with which the workshop is charged, seeking to construct a definition that satisfies the group and which sets the parameters within which the specific issues, activities, or tasks are identified. A set of criteria for measuring success are also identified. Group discussion clarifies the identified issues and leads to consensus on their definition and scope. The issues are then relatively ranked (that is, the items in the set are ranked against each other, and not against any external, absolute standard) using pair-wise comparisons that compare each issue to all others in the set in turn against each of the identified selection criteria by asking the scorer to assign specific values to each issue. This forces panelists to make explicit the tradeoff process and the criteria by which they are making the tradeoffs.

APPENDIX D

RESULTS FROM PRE-WORKSHOP QUESTIONNAIRE TO INDUSTRIAL PARTICIPANTS

Critical Needs and Evaluation Criteria Questionnaire for Industrial Participants Catalyst Roadmapping Workshop

This questionnaire will be used as a starting point for our discussion at the workshop involving the ranking of catalyst research needs for chemical synthesis and the criteria that should be used to select catalyst research investment areas. Below are the critical needs for catalysis identified by the Council for Chemical Research Chemical Synthesis Committee. Please rank in order of importance (1 being the most important) and add any additional MAJOR critical needs for catalysis research your company has identified.

- ___ Simple techniques for rapid throughput catalyst synthesis with a focus on molecular diversity, i.e. a wide range of catalyst compositions
- ___ Clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation
- ___ Better in situ techniques for catalyst characterization
- ___ Enable rational catalyst design through combined mechanistic understanding and improved computational chemistry
- ___ Development of techniques to prepare supported homogeneous catalysts
- ___ Exploitation of interfaces of chemical synthesis with biotechnology and material science
- ___ Development of multi-step, "one pot" reactions
- ___ Identification of new approaches to big stake areas such as selective oxidation, solid acid/base catalysis, living polymerizations, functional olefin polymerization

Additional MAJOR critical needs _____

Rank the evaluation criteria suggested below for research investments (1 being most important):

- ___ Impact of technology advances
 - ___ Timeliness of the impact of technology advances
 - ___ Probability of successful technology development
 - ___ Cost of investment relative to the potential benefit of the technological advance
 - ___ Appropriateness of a government role in developing associated advanced technologies
- Please suggest what would or would not be an appropriate role for government research investment in catalysis (add additional page if needed): _____

Additional evaluation criteria suggestions: _____

Please feel free to send any additional comments or suggestions.

RESULTS FROM PRE-WORKSHOP QUESTIONNAIRE

The questionnaire on the previous page was sent to all industrial invitees. In addition to the Workshop participants, invited companies included Union Carbide, Eastman Chemical, Exxon Chemical, Shell Chemical, Hoescht, Merck, Pfizer, PQ, WR Grace, Proctor and Gamble, Catalytica and SRI. There was no attempt to take a scientific survey, the workshop organizers were just interested in getting additional ideas and developing a broad-based straw man for the workshop to use as a starting point. Questionnaire results represent individual opinions and not companies. More than one completed questionnaire was received from some of the companies.

The critical needs were ranked by order of importance. The total number of points is given in Table D1 below.

Table D1. Critical needs in order of ranking by industrial questionnaire participants

CRITICAL NEEDS IN ORDER OF RANKING	WEIGHTED VOTING
Identification of new approaches to big stake areas such as selective oxidation, solid acid/base catalysis, living polymerizations, functional olefin polymerization	16
Enable rational catalyst design through combined mechanistic understanding and improved computational chemistry	15
Better in situ techniques for catalyst characterization	14
Simple techniques for rapid throughput catalyst synthesis with a focus on molecular diversity, i.e. a wide range of catalyst compositions	11
Development of techniques to prepare supported homogeneous catalysts	11
Clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation	11
Development of multi-step, "one pot" reactions	11
Exploitation of interfaces of chemical synthesis with biotechnology and material science	11

Additional critical needs suggested by industrial participants through the questionnaire are listed below.

- Synthesis and characterization of catalyst supports
- More efficient product separation techniques
- Better methods for testing long term catalyst activity
- Better sulfur-resistant catalysts
- Catalysis for waste remediation
- Asymmetric catalysts with high turnover

- Non steady-state catalysis

Criteria for ranking the critical needs were ranked as shown in Table D2.

Table D2. Industrial questionnaire response on criteria for ranking critical needs in catalysis

CRITERIA FOR RANKING CRITICAL NEEDS	RELATIVE RANKING
Impact of technology advances	29
Cost of investment relative to the potential benefit of the technological development	24
Timeliness of the impact of technology advances	19
Probability of successful technology development	15
Appropriateness of a government role in developing associated advanced technologies	14

Comments were given by industrial respondents regarding the appropriate role for government research investment in catalysis. Two comments were made by many of the respondents and are listed below:

1. Not appropriate for government to work on specific catalysts/processes for proprietary products
2. Should fund breakthrough, precompetitive research.

One respondent thought it was not appropriate to build a large government catalysis institute and that it was appropriate to fill the research gap between academia and industry.

APPENDIX E

RESULTS FROM POST-WORKSHOP QUESTIONNAIRE TO WORKSHOP PARTICIPANTS

RESEARCH INVESTMENT RANKING

POST-WORKSHOP SURVEY

Since the groups which identified the research investments for each critical need were quite small (9-11), the workshop decided to send a questionnaire to all workshop participants requesting that they rank the research investments identified by all the subcommittees for each of the four major critical needs. A copy of the questionnaire is included at the end of Attachment E. Twenty participants responded to the questionnaire and this included 10 industrial representatives, seven academic participants, and three national laboratory participants. Their responses are tabulated below.

The ranking information on the three major research investments for the first critical need, Enable catalyst design through combined experimental, mechanistic understanding and improved computational chemistry, is listed in Figure 1E below. Note that the post-workshop ranking is different than the subgroup ranking. Working on high impact areas did not seem as important to the larger group in retrospect than it did to the subgroup during the workshop. The first two investments are broken down into further research investments and the rankings are listed in Figures 2E and 3E.

Figure 1E. Enable catalyst design through combined experimental, mechanistic understanding, and improved computational chemistry

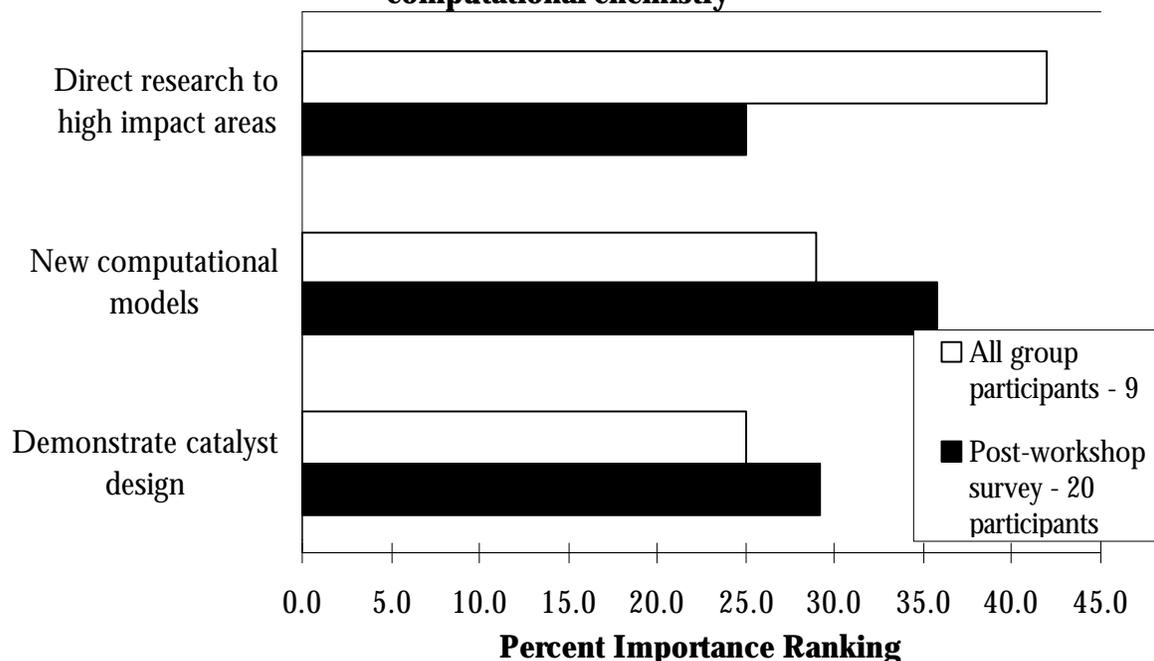


Figure 2E. Conduct experiments directed towards high impact areas, especially these four types of studies

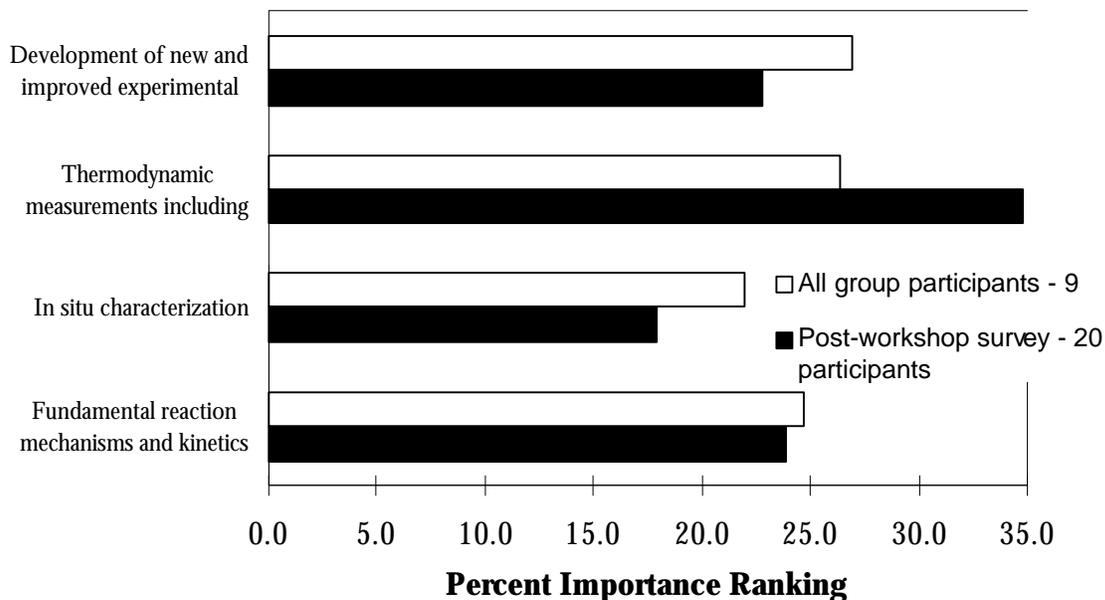
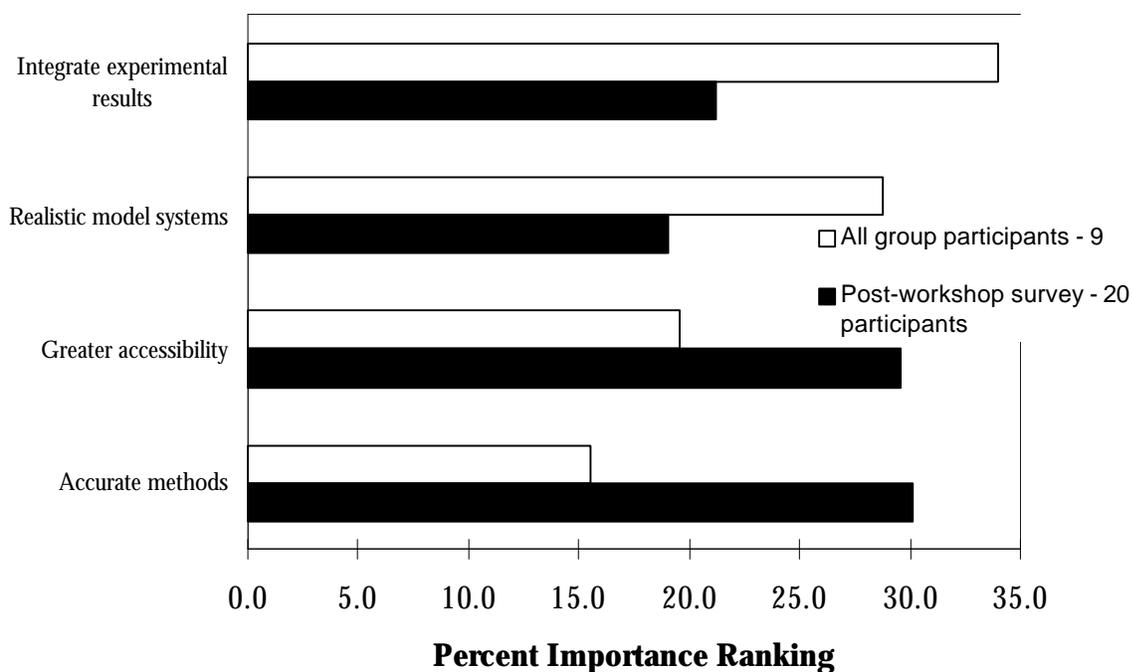


Figure 3E. Develop new or improved computational chemistry models with emphasis on the following



The rankings for the research investments for the second through fourth critical need are summarized in Figures 4E-6E.

Figure 4E. Development of techniques for high throughput synthesis of catalysts and clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation.

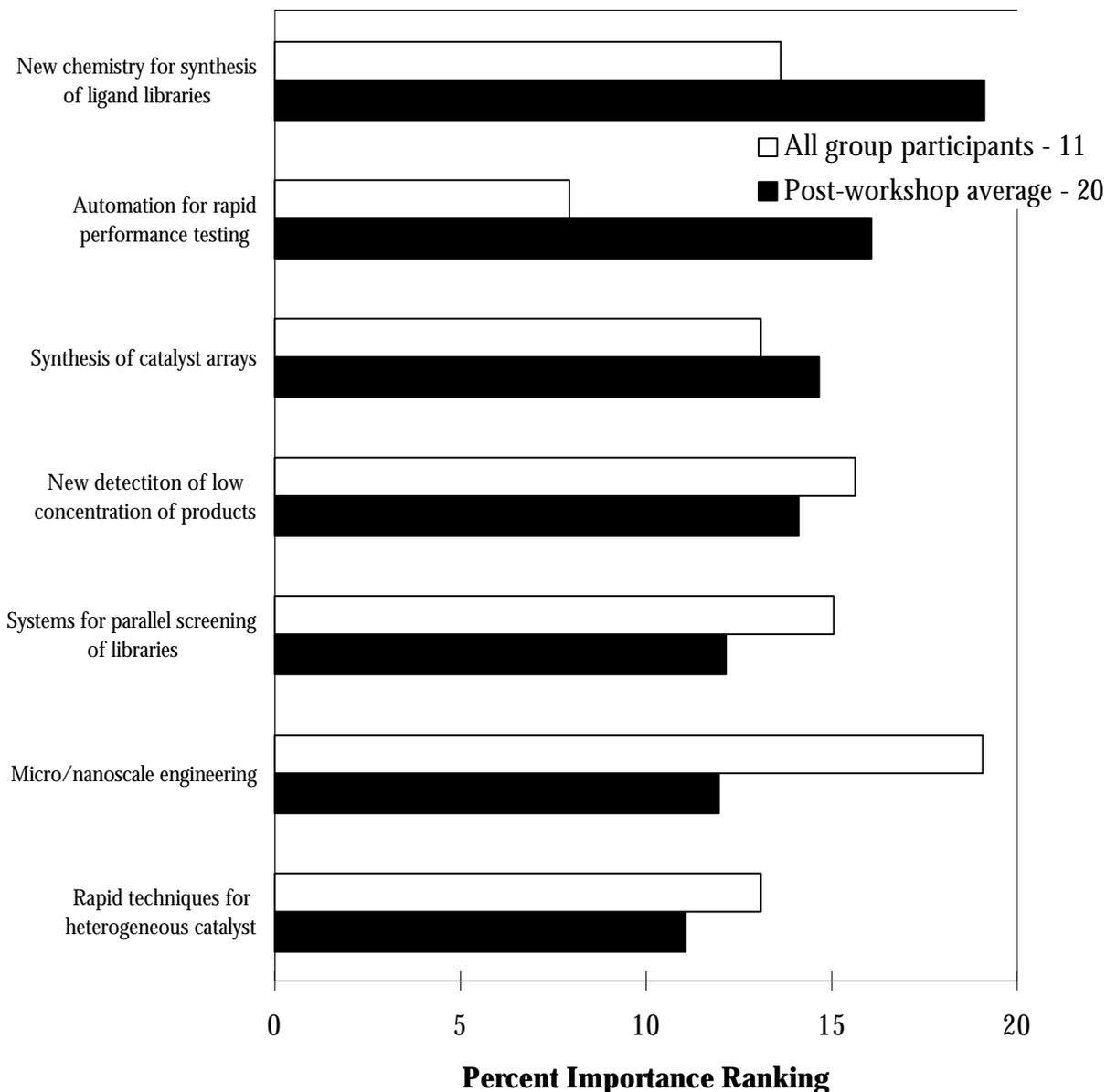


Figure 5E. Better in situ techniques for catalyst characterization

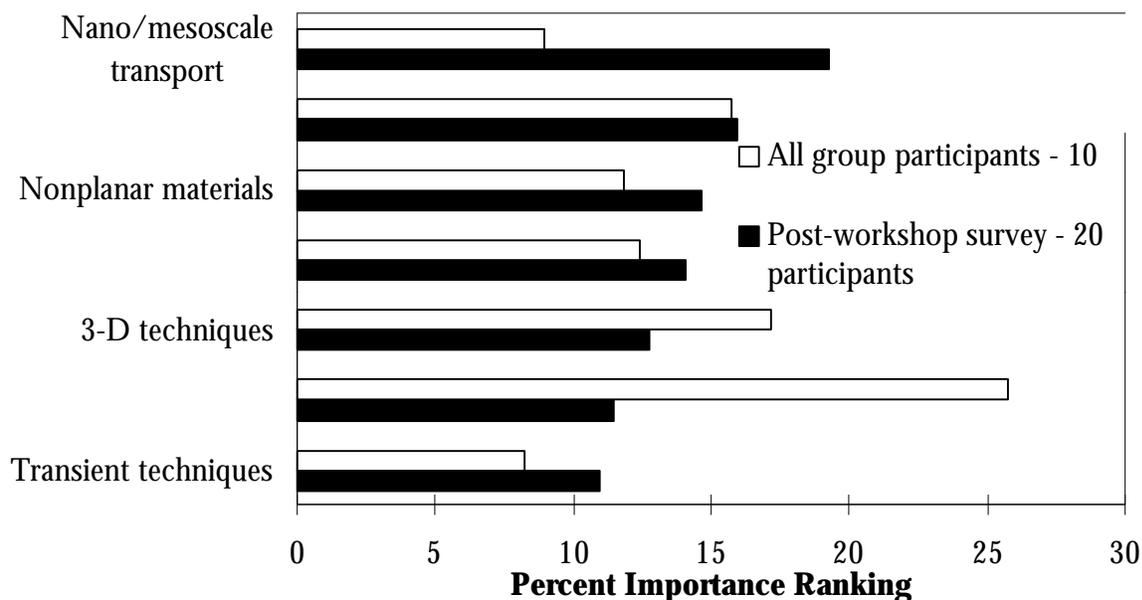
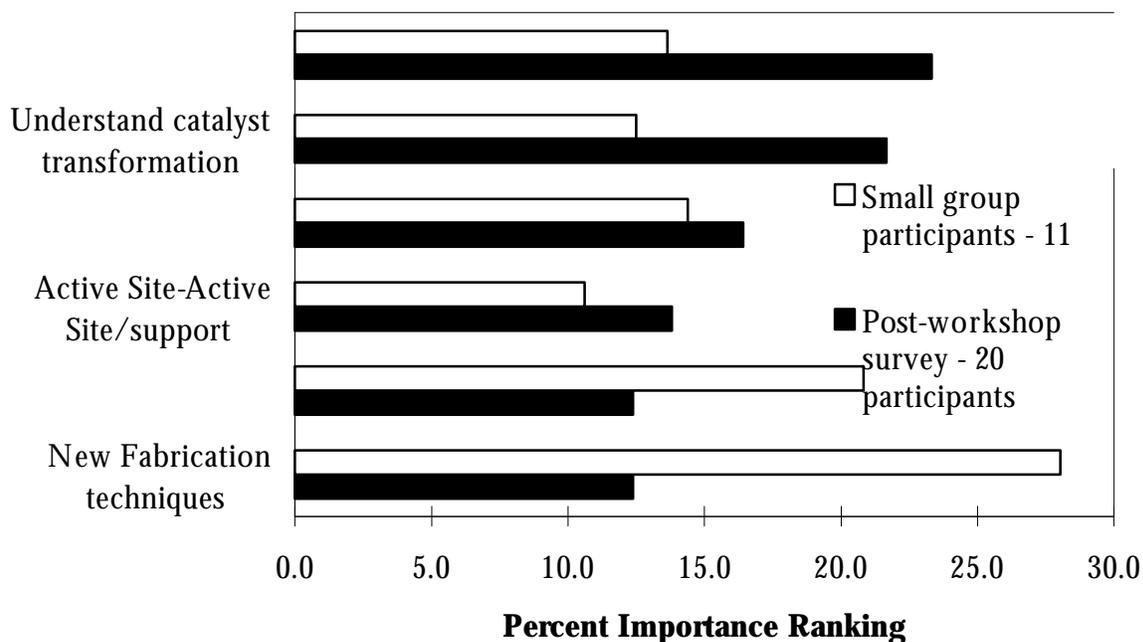


Figure 6E. Synthesis of catalysts with specific site architecture



Post Workshop Ranking of Research Investment

Name _____

Affiliation _____

Please refer to Catalyst Technology Roadmapping Draft Report for background information on the four critical needs.

1. **Enable catalyst design through combined experimental, mechanistic understanding, and improved computational chemistry.**

Please indicate whether you think each research investment is a **short (3-5 years) S**, **medium (6-9 years) M** or **long (>9 years)L** investment or some combination of the three.

RANK THE THREE MAJOR TOPICS (IN CAPS) BELOW 1-3 (**1 IS MOST IMPORTANT**.)

____ CONDUCT EXPERIMENTS DIRECTED TOWARDS HIGH IMPACT AREAS, ESPECIALLY THE FOLLOWING TYPE OF STUDIES

Rank the four items below 1-4

- Thermodynamic measurements including adsorption and desorption studies, surface reaction studies, and transient species
- Fundamental reaction mechanistic and kinetic studies
- In situ characterization studies
- Development of new and improved techniques with greater temporal, spatial, and species resolution

____ DEVELOP NEW OR IMPROVED COMPUTATIONAL CHEMISTRY MODELS WITH EMPHASIS ON THE FOLLOWING

Rank the four items below 1-4

- More realistic model systems incorporating complexities of real catalysts such as medium effects and realistic cluster sizes
- More accurate methods
- Methods that better integrate with experimental results in areas such as thermochemistry, kinetics, transport properties, and phase
- Methods with greater accessibility for the broader scientific community

____ DEMONSTRATE CATALYST DESIGN FROM THE COMBINATION OF EXPERIMENTAL, COMPUTATIONAL, AND MECHANISTIC KNOWLEDGE

2. Development of techniques for high throughput synthesis of catalysts and clever new assays for rapid throughput catalyst testing, potential combinatorial techniques, and reduction of analytical cycle time by parallel operation and automation.

Rank the 7 items below 1-7. (1 is most important.)

Please indicate whether you think each research investment is a **short (3-5 years) S**, **medium (6-9 years) M** or **long (>9 years)L** investment or some combination of the three.

___MICRO- AND NANO-SCALE ENGINEERING

___NEW APPROACHES FOR RAPID DETECTION OF LOW CONCENTRATION OF PRODUCTS

___SYSTEMS FOR PARALLEL SCREENING OF LIBRARIES, PARTICULARLY UNDER DIFFICULT CONDITIONS INCLUDING HIGH TEMPERATURES AND PRESSURES, STRICTLY ANAEROBIC ENVIRONMENTS

___NEW CHEMISTRY FOR SYNTHESSES OF LIGAND LIBRARIES

___SYNTHESIS OF CATALYST ARRAYS WITH HIGH SPATIAL RESOLUTION

___RAPID TECHNIQUES FOR DETAILED CHARACTERIZATION OF HETEROGENEOUS CATALYST LIBRARIES

___AUTOMATION FOR RAPID PERFORMANCE TESTING

3. Better in situ techniques for catalyst characterization

Rank the 7 items below 1-7. (1 is most important.)

Please indicate whether you think each research investment is a **short (3-5 years) S**, **medium (6-9 years) M** or **long (>9 years)L** investment or some combination of the three.

___DEVELOPMENT OF X-RAY SPECTROSCOPIES (INCLUDING ABSORPTION) AND X-RAY MICROSCOPY WITH HIGHER SPATIAL, TEMPORAL, AND ENERGY RESOLUTION -

___THREE-DIMENSIONAL TECHNIQUES (PET, MAGNETIC RESONANCE IMAGING, AND NMR SPECTROSCOPY)

___SCANNING PROBES OR MOLECULAR REPORTERS SUCH AS RADIOTRACERS -

___IN SITU DIFFRACTION AND MICRO-DIFFRACTION TECHNIQUES -

___DEVELOPMENT OF TECHNIQUES FOR NONPLANAR AND ROUGH MATERIALS

___TECHNIQUES FOR NANO/MESOSCALE TRANSPORT MEASUREMENT FOR MODEL VERIFICATION

___TRANSIENT TECHNIQUES FOR MEASUREMENT OF PHYSICAL (E.G. THERMODYNAMIC) PROPERTIES, AND THEIR EVOLUTION IN SITU

4. Synthesis of catalysts with specific site architecture

Rank the 6 items below 1-6. (1 is most important.)

Please indicate whether you think each research investment is a **short (3-5 years) S**, **medium (6-9 years) M** or **long (>9 years)L** investment or some combination of the three.

___NEW FABRICATION METHODS FOR CATALYSTS

___TECHNOLOGY DEVELOPMENT TO DESCRIBE/CHARACTERIZE SOLID ACTIVE SITE AT ATOMIC LEVEL

___UNDERSTAND/SYNTHESIZE MULTI-CATALYST SYSTEMS

___TECHNOLOGY TO ACCELERATE AGING MEASUREMENTS

___DESCRIBE CHEMICAL TRANSFORMATION OR THE WAY A CATALYST PHASE ASSEMBLES (E.G., SOL TO CRYSTAL FORMATION)

___UNDERSTAND ACTIVE SITE-ACTIVE SITE AND ACTIVE SITE-SUPPORT INTERACTIONS

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