Future Directions in Surface Catalysis

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Catalysis by solid surfaces is central to the technology of conversion of fuels; abatement of pollution; and synthesis of chemicals, pharmaceuticals, fertilizers, polymers, and nanomaterials. It seems almost inevitable that catalysis will increase markedly in importance in all of these applications. This presentation is meant to provide a summary of thoughts about where the field may be going on the basis of perceived needs for improved control of chemical conversions and recent advances in research that are advancing catalysis and related fields.

The largest-scale applications of catalysis are in fuel production and pollution abatement. With the energy and environmental challenges the world faces and the increasing realization of these challenges, it is evident that we need major innovations in both of these directions, and catalysis must be at the center.

Challenges in fuel conversion dictate the control of transformation of markedly heavier and dirtier fossil fuels, including heavy oil, oil-sands-derived liquids, coal-derived liquids, and shale-derived liquids; biomass also offers potentially significant sources of renewable fuels that must be assessed. The existing catalysts for heavy petroleum conversion provide a good starting point for the next generation of fossil fuel conversion processes, but much improved catalysts will be needed. It is essential that a detailed molecular understanding of the feedstocks be developed so that the various competing reactions can be elucidated and catalysts can be found that are tailored for specific feedstocks and feedstock fractions, to be converted in the presence of components that cause rapid deactivation of today's catalysts. The need for analytical chemistry of the complex feedstocks as part of the needed research in catalysis seems likely to set the research in these directions apart from earlier research in fossil fuel conversion.

Biomass conversion catalysis is in its infancy, and it is difficult to assess its prospects for economic application. The high oxygen content of biomass leads to new challenges in catalysis, as the reaction pathways and catalyst deactivation phenomena are qualitatively different from those of almost all existing processes and will seemingly require classes of catalysts that are essentially different from today's.

Conversion of effluents from motor vehicles and power plants has become extremely effective and provides a strong demonstration of the social value of catalysis, but innovations are needed to facilitate catalytic solutions of the challenge of converting CO_2 formed in fossil fuel conversion and converting water into H_2 and O_2. The needs suggest opportunities for photocatalysis and processes emulating photosynthesis, and the prospects of high-temperature catalysis are also tantalizing, but largely unexplored.

Extensive research will be needed for landmark advances in these directions. The opportunities for major advances in research are excellent, facilitated by continuing rapid advances in experimental methods of surface characterization and theory and computation, bolstered by novel methods of materials synthesis. Exploitation of the improving and emerging scientific tools, at least in the U.S., will require a funding base that is far stronger than today's.

Understanding of catalysis on surfaces is challenging because surfaces of most catalysts are dauntingly complex and nonuniform and work at high temperatures and often high pressures—and because the catalytically active species are small and dispersed within solids and difficult to characterize. Most of the reported experimental results characterizing catalysts represent them under conditions far removed from those of catalysis—so that the structures investigated are often not entirely relevant to catalysis.

The techniques for investigation of catalysts in reactive atmospheres continue to improve markedly and rapidly—the application of spectroscopic and even microscopic techniques to working catalysts is a major trend in recent research and is likely to continue strongly.

Fundamental understanding of solid catalysts is increasingly expected to emerge from investigations of catalysts that are structurally uniform—the successors of single crystals of metal, such as well-made zeolites—so that the catalytic sites constitute uniform arrays. This class of catalytic material can be extended by anchoring analogues of homogeneous catalysts ("molecular" species) onto solids with uniform surfaces, so that the characterization by spectroscopy can be incisive and theory can be applied with a rigor approaching that in molecular chemistry.

What's more, it is becoming possible to investigate individual catalytic species (nanoparticles) in the presence of many other species, and we may anticipate further progress in this direction. Such results will set a foundation for truly fundamental understanding of how individual catalytic species work, even in highly complex catalytic materials. Some day, we envision single-molecule spectroscopy for characterization of molecules reacting on individual catalyst structures. Ultimately such results will allow elucidation of truly fundamental structure-performance relationships in catalysis, so that the results can be integrated over whole, complex catalysts.