Proceedings of the Fifth Meeting on Basic Heterogeneous Catalysis Surface Science Research

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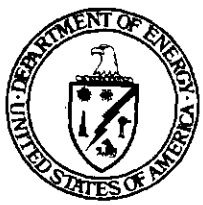

U.S. Department of Energy
Office of Basic Energy Sciences
Office of Chemical Sciences
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TABLE OF CONTENTS

DOE

HETEROGENEOUS CATALYSIS RESEARCH MEETING

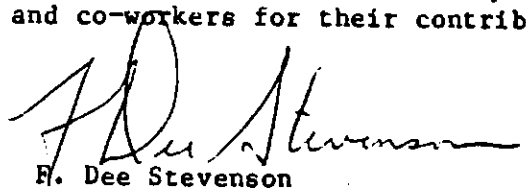
Office of Basic Energy Sciences

1. Introduction

This report summarizes the proceedings of the fifth DOE/BES meeting on basic heterogeneous catalysis and surface science research which was jointly sponsored by the Division of Chemical Sciences and the Division of Materials Sciences. Participants in this meeting included researchers from the DOE Laboratories, University researchers currently receiving BES support for catalysis and/or surface science research, and representatives from DOE Headquarters Divisions.

The meeting was held primarily to (1) acquaint each participant, including the DOE administrative staff, with the research being currently supported, (2) to identify the most recent notable accomplishments, and (3) to focus attention on the needed but unanswered technical and scientific questions. Because of time limitations, only part of the principal investigators present were able to give a review of their research.

Following the presentations, the industrial representatives commented on industrial research needs, after which there was a discussion on surface science and its potential contribution to catalysis. Summary of the discussion period was prepared by Dr. Robert P. Eischens of the Division of Chemical Sciences and is included in the Summary of this report. Brief project summaries constitutes the balance of this report. Special thanks go to Bob Eischens for organizing this meeting and for the report summary and, also, to each participant and co-workers for their contributions.



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Discussion Summary

Because of the direct relationship between heterogeneous catalysis and energy, and because of the scientific opportunities in this field, support of basic catalysis research by DOE's Office of Basic Energy Sciences has expanded significantly during the last decade. Currently this large and diverse catalysis program is a representative cross section of the goals and accomplishments of basic catalysis researchers in the United Stated. Forty-six research descriptions were submitted for the meeting. There was not sufficient time for oral presentations on all of the projects. Therefore emphasis was placed on topics such as metal-support interactions and surface science where the numbers of projects warranted mini-symposia to be organized within the overall meeting format.

Metal-support interactions have been of interest since G.-M. Schwab focussed attention on this concept about four decades ago. Schwab limited the definition of metal-support effect to cases where the support was a semiconductor, such as alumina, and the effect could be attributed to transfer of electrons at the metal-semiconductor interface. This definition excluded effects due to differences in the particle size of the supported metal or to formation of difficultly reduced mixed oxides. Over the intervening years there were many examples of the modification of catalytic activity of supported metals. However, none of these examples were sufficiently well established to be widely accepted as attributable to metal-support effects as defined by Schwab. This was changed by Tauster's discovery of the modification of platinum on titania which he attributed to electron transfer although not precisely in the semiconductor-metal context as visualized by Schwab. Most of the metal-support effect presentations in the meeting directly, or by implication, were based on acceptance of Tauster's electron transfer mechanism. However, Henrich reported results suggesting that, under strong reducing conditions, rhodium disappears from the surface of Rh/TiO_2 samples by diffusion of the rhodium into the support or by migration of the support over the surface of the rhodium. This mechanism would not be considered a metal-support effect so the question of metal-support interactions is not yet satisfactorily answered.

Representatives of industry were invited to attend the meeting and participate in the discussions. The discussion of "An Industrial View of Current Catalysis Research" benefited from the productive contributions of John Larson, Mordecai Shelef, Sam Tauster, John Peri, and Mike Kelley. The objective of the BES catalysis program is to gain information pertinent to and understanding of the fundamental aspects of catalysis rather than attempting to discover and develop better catalysts. The concensus of the industrial representatives was in accord with this concept of the proper role of BES sponsored research.

The discussion of which types of surface science are of most value to catalysis research was led by Alex Bell, Dave Hercules, John Yates, and Marv Poutsma. Specific support was given to the need to study catalyst surfaces while reactions are in progress. The vibrational spectroscopies, infrared and Raman, are most easily applicable to such studies. Electronic spectroscopies, such as Auger and XPS, were cited as having special utility because they could be applied to practical catalysis such as used for hydrodesulfurization. Marv Poutsma indicated that solid state NMR has a promising potential in catalysis studies. There was general agreement with this evaluation of the potential of NMR.

Two of the objectives of this series of heterogeneous catalysis meetings have been to acquaint industrial researchers with the BES program and to expose the BES sponsored investigators to the views of catalysis experts from industry. Because of the limited emphasis on publication of industrial work, it is difficult for academic researchers to become aquainted with the science underlying the strengths of the nations industrial catalysis effort. These strengths have led to the development of some of the world's greatest industries and have made possible American leadership in catalysis. Academic institutions have contributed by providing the sophisticated trained manpower which is essential for successful industrial research. As not constituted, DOE grants for academic research appear to be sufficiently flexible to support exposure of faculty and students to work in industrial laboratories for periods of a few months. It is hoped that methods can be devised to utilize such temporary transfers to improve the interaction between industrial and academic catalysis workers.

Earl Muetterties was scheduled to make a presentation at this meeting. He made many significant contributions to DOE catalysis programs and gave promise of many more. He will be sorely missed.

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