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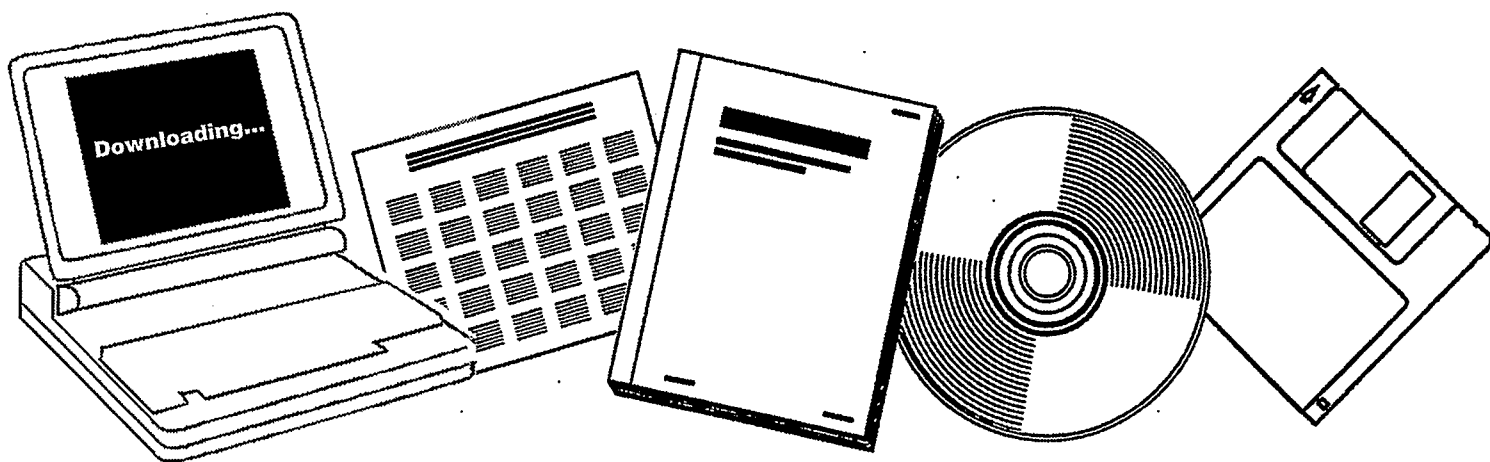
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STUDY OF CRYSTALLITE SIZE AND SUPPORT INTERACTIONS ON CO HYDROGENATION

PENNSYLVANIA STATE UNIV., UNIVERSITY
PARK. DEPT. OF CHEMICAL ENGINEERING

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A Study of Crystallite Size and Support
Interactions on CO Hydrogenation

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Progress Report

to the

Division of Chemical Sciences
Office of Basic Energy Research
U.S. Department of Energy

by

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Accomplishments (1980-1982)

The past year and a half has been spent primarily adapting a differential scanning calorimeter so that support effects on isothermal heats of adsorption can be measured directly. I know of no other similar investigation utilizing such instrumentation although Gravelle and coworkers have been studying metal alloys using a non-flow calorimeter (24). In addition, we now believe that temperature programmed desorption (TPD) studies can also be conducted with our experimental system, and our present design is shown in Figure 1. It presently provides flows of Ar, H₂, and CO and mixtures thereof, and allows both in situ pretreatment and TPD studies as the desorption endotherm is monitored to follow the desorption process. Initial results for H₂ are shown in Figure 2, which are consistent with previous reports using different techniques (25-27) and they illustrate this type of calorimeter has the necessary sensitivity to provide satisfactory data. The most persistent problem has been baseline perturbation due to variations in gas mixtures and gas flow rates through the sample and reference cells. The incorporation of flow controllers from funds external to this program has alleviated the first problem, but additional controllers are needed to minimize the second.

The in situ IR system has been upgraded by again using funds external to this study and adding an Apple II Plus computer with floppy disc storage, a TV set, and a printer/plotter along with the necessary software. Having been forced to modify the IR cell design by King (28), which did not work due to unacceptable air leaks, we are now conducting our first set of transient studies on Pt/Al₂O₃ and Pt/TiO₂ catalysts.

During the past two years, research sponsored by this program has resulted in seven papers presented at national meetings, two papers presented at international meetings, and twelve invited lectures presented at different universities and companies. Five additional papers have been published, one manuscript has been submitted for publication, and two are in the final stages of preparation.

Since September 1, 1980, two students have received their Ph.D. degrees, one student received his M.S. degree, and another student should graduate with his M.S. degree before August, 1982. One student is currently working on the project and another Ph.D. student is planning to join the program this summer.

List of Publications Since Sept. 1980

Smith, J. S., Thrower, P. A., and Vannice, M. A. Characterization of Ni/TiO₂ Catalysts by TEM, X-Ray Diffraction, and Chemisorption Techniques. J. Catal. 68, 270 (1981).

Vannice, M. A. and Wang, S-Y., Determination of IR Extinction Coefficients for Linearly - and Bridged-Bonded CO on Supported Palladium, J. Phys. Chem. 85, 2543 (1981).

Vannice, M. A., Moon, S. H., and Wang, S-Y., The Effect of SMSI Behavior on CO Adsorption and Hydrogenation on Pd Catalysts, Part I - IR Spectra of Adsorbed CO Prior To and During Reaction Conditions. J. Catal. 71, 152 (1981).

Wang, S-Y., Moon, S. H. and Vannice, M. A. Part II - Kinetic Behavior in the Methanation Reaction. J. Catal. 71, 167 (1981).

Vannice, M. A. and Twu, C. C., Extinction Coefficients and Integrated Intensities for Linear - and Bridged-Bonded CO on Platinum, J. Chem. Phys. 75, 5944 (1981).

Vannice, M. A., Twu, C. C., and Moon, S. H., "SMSI Effects on CO Adsorption and Hydrogenation on Pt Catalysts", J. Catal. - Submitted for publication.

Reprints of the above publications have been sent directly to Dr. Stevenson, Division of Chemical Sciences.