Probing Catalyst Structure-Performance Relationships through Studies of Reaction Mechanism and Kinetics

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An enduring challenge for the field of catalysis is to understand how catalyst composition and structure are related to catalyst activity and selectivity. The achievement of this goal requires knowledge of what is meant by a catalytically active center, the mechanism by which reactants are converted to products, and the kinetics of the elementary processes appearing in the mechanism. Modern analytical methods enable the characterization of catalysts at the level of atoms and molecules. It is also possible to probe the mechanism of catalyzed reactions through use of various transient response methods and thereby elucidate the most likely elementary processes by which reactants are converted to products. Equally important is the use of modern theoretical methods to verify the structures of active centers deduced from experiments and to assess whether elementary processes proposed on the basis spectroscopic and other means are plausible. This talk will illustrate how various experimental and theoretical methods can be used both separately and in combination to achieve a deep understanding of the factors controlling catalyst activity and selectivity. It will also be shown how such understanding can be used to guide the development of a more active and selective catalyst. The examples discussed will include the decomposition of N_2O, the oxidation of methanol, the synthesis of methanol, and the epoxidation of olefins.