Preface

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This volume of *Topics in Catalysis* entitled “Catalyst Characterization by Vibrational Spectroscopy” is dedicated to the memory of Helmut Knözinger, a passionate catalysis researcher and surface spectroscopist, who made significant contributions in several areas of catalysis by developing and by applying characterization methods. Helmut Knözinger passed away in January 2014, after a long and successful career as university professor in Physical Chemistry, as detailed by Che, Ertl, Hadjiivanov and Gates in *Advances in Catalysis* 57 (2015) xi. He began his higher education with studies in Physics at Ludwig-Maximilians-Universität München, where he obtained his doctoral degree in 1961 and completed his habilitation in 1967. He continued his career at LMU and became Professor in 1980. While Helmut Knözinger engaged in numerous collaborations near and far and visited many research laboratories around the world, he stayed true to his Alma Mater throughout his active career and even past retirement.

The intent of this volume is to highlight the methods and methodologies that Helmut Knözinger developed and applied for the characterization of surface sites and surface species, together with the associated catalysis research themes. The volume begins with a personal review of Knözinger’s major contributions to catalysis and surface spectroscopy written by Gerhard Ertl. The volume continues with

articles by experts that demonstrate how the characterization methods used by Knözinger are applied and further developed today.

The first block of six of articles focuses on the characterization of the surfaces of solid acids and bases and their reactivity. Infrared spectroscopy and the application of probe molecules are central to the analysis of the structures present or forming on the surface, and to the measurement of acidic and basic properties. Two articles in this group, one a review by Hadjiivanov and co-workers and one an original article by Kondo and co-workers, take advantage of the insight provided by isotopes. Dobrotvorskaia and Tsyganenko address the influence of lateral interactions of probe molecules on the spectral signature. Weckhuysen and co-workers investigate hydroxyapatite catalysts under operating conditions, an approach supported by Knözinger by dedicating three volumes of *Advances in Catalysis* to this methodology. In the subsequent three articles, aluminum is the key element for the generation of surface acidity. Hunger, Busca, and Beutel and their co-workers use infrared and other spectroscopies to characterize the sites on the surface of mixed oxides containing aluminum and silicon or titanium.

The second block of six articles is devoted to the characterization of dispersed ionic transition metal species. Abatement of NO_x is an important application of this type of catalysts. One type of species are oxide-supported oxometallates of early transition metals whose structures lend themselves to characterization by Raman spectroscopy. Wachs and co-workers open this section with a summary of the spectral information that has been accumulated in the literature, followed by original contributions of Stair and Hess and their co-workers on supported molybdate and vanadate species. A second type of species in this block are cations of late transition metals incorporated into zeolitic materials, which are characterized by reactive or nonreactive interaction with

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probe molecules and IR spectroscopy. Bentrup, Concepcion, Bordiga and their respective author teams report on the state and reactivity of iron, copper, and nickel cations.

A third block of three articles is dedicated to the analysis of the bulk structure of metal oxides, which is accomplished by Raman spectroscopy. Reddy and co-workers report on nanostructured and doped ceria. In a series of two papers on vanadyl pyrophosphate, Wintterlin, Mestl, Rösch and their co-workers provide structure–activity relationships and computational insight into maleic anhydride formation.

The volume concludes with a block of four papers on the nature and behavior of supported metal particles, which are characterized by IR spectroscopic analysis of small adsorbed molecules. Azzolina-Jury and Thibault-Starzyk describe plasma-assisted CO₂ hydrogenation on nickel, and Föttinger et al. report on the formation of carbonates on alumina-supported palladium. The last two articles are concerned with

strong interactions between support and metal and the role of the metal-support interface. Trunschke and co-workers monitor the surface composition of a copper and zinc oxide catalyst during methanol synthesis, whereas Strunk and co-workers focus on the gold-titania interface and its role as a nucleation point for support reduction.

In sum, the articles in this volume demonstrate that methods based on vibrational spectroscopy continue to be applied by many researchers in the field of catalysis. Advances have been made in the application under operating conditions and in the interpretation of spectral data. A wealth of reference spectra have been accumulated in the literature, facilitating assignments. The wide range of materials and the large variety of scientific questions addressed confirm what Helmut Knözinger opined: it is always worthwhile to do a spectroscopic experiment.