

Structure Activity And Selectivity Relationships In Heterogeneous Catalysis

Past and Present in DeNO_x Catalysis: From Molecular Modelling to Chemical Engineering - Pascal Granger 2007-12-15

This book offers an overview of the state of the art in the field of DeNO_x catalysis in order to focus novel orientations, new technological developments, from laboratory to industrial scale. A particular attention has been paid towards the implementation of catalytic processes for minimising NO_x emissions either from stationary or mobile sources under lean condition to meet future standard regulations of NO_x emissions. In the first part of this book, critical aspects reported in the literature which usually make difficult the achievement of efficient catalytic technologies in those conditions are summarised and analysed in order two separate new perspectives. The second part deals with fundamental aspects at molecular level. A better understanding of the reactions involved under unsteady-state conditions is probably a pre-requisite step for improving the performances of the actual processes or developing original ones. The development of powerful in situ spectroscopic techniques is of fundamental interest for kinetic modelling. Correlations between spectroscopic and kinetic data with those obtained from theoretical calculations are reported. Some illustrations emphasise the fact that these comparisons may help in determining the nature of the catalytic active sites and building predictive tools for simulations under running conditions. The latter part of this book will be illustrated by different practical approaches covering various aspects related to the catalysts preparation and the development of alternative technologies which include industrial considerations. - New technological developments for investigating catalytic reactions in transient conditions

(in situ and operando spectroscopic techniques) - Concerted approaches in DeNO_x catalysis - How academic aspects (kinetic, in situ spectroscopic measurements) can provide useful information for practical applications - Comparison of different approaches provided by academic and industrial partners

Structure-Activity and Selectivity Relationships in Heterogeneous Catalysis - R.K. Grasselli 1991-07-09

Structure plays an important role in heterogeneous catalysis. It provides a framework for the arrangement and strategic placement of key catalytic elements, hosting them in a prescribed manner so that their respective electronic properties can exhibit their desired catalytic functions and mutual interactions. Under reaction conditions these framework structures and their catalytic guests undergo dynamic processes becoming active participants of the overall catalytic process. They are not mere static geometric forms. The dynamics of catalytic structures are particularly vivid in selective oxidation catalysis where the lattice of a given catalytic solid partakes as a whole, not only its surface, in the redox processes of the reaction. The catalyst becomes actually a participating reagent. By proper choice of key catalytic elements and their host structures, preferred catalytic pathways can be selected over less desired ones. However, not only in selective redox catalysis does structure play an important role, its importance is also well documented, among others, in shape selective zeolite catalysis, enantioselective hydrogenation and hydrodesulfurization. The contributions presented in this book address the dynamic character of the solid state under catalytic reaction conditions. By relating structure to activity and selectivity in

heterogeneous catalysis our understanding of such correlations has been significantly enhanced through the use of sophisticated spectroscopic means, surface science and modeling.

Selective Oxidation by Heterogeneous Catalysis - Gabriele Centi
2012-12-06

Selective Oxidation by Heterogeneous Catalysis covers one of the major areas of industrial petrochemical production, outlining open questions and new opportunities. It gives keys for the interpretation and analysis of data and design of new catalysts and reactions, and provides guidelines for future research. A distinctive feature of this book is the use of concept by example. Rather than reporting an overview of the literature results, the authors have selected some representative examples, the in-depth analysis of which makes it possible to clarify the fundamental, but new concepts necessary for a better understanding of the new opportunities in this field and the design of new catalysts or catalytic reactions. Attention is given not only to the catalyst itself, but also to the use of the catalyst inside the process, thus evidencing the relationship between catalyst design and engineering aspects of the process. This book provides suggestions for new innovative directions of research and indications on how to reconsider the field of selective oxidation from different perspectives, outlining that is not a mature field of research, but that new important breakthroughs can be derived from fundamental and applied research. Suggestions are offered on how to use less conventional approaches in terms of both catalyst design and analysis of the data.

Catalysis by Materials with Well-Defined Structures - Zili Wu 2015-03-26
Catalysis by Materials with Well-Defined Structures examines the latest developments in the use of model systems in fundamental catalytic science. A team of prominent experts provides authoritative, first-hand information, helping readers better understand heterogeneous catalysis by utilizing model catalysts based on uniformly nanostructured materials. The text addresses topics and issues related to material synthesis, characterization, catalytic reactions, surface chemistry, mechanism, and theoretical modeling, and features a comprehensive review of recent

advances in catalytic studies on nanomaterials with well-defined structures, including nanoshaped metals and metal oxides, nanoclusters, and single sites in the areas of heterogeneous thermal catalysis, photocatalysis, and electrocatalysis. Users will find this book to be an invaluable, authoritative source of information for both the surface scientist and the catalysis practitioner Outlines the importance of nanomaterials and their potential as catalysts Provides detailed information on synthesis and characterization of nanomaterials with well-defined structures, relating surface activity to catalytic activity Details how to establish the structure-catalysis relationship and how to reveal the surface chemistry and surface structure of catalysts Offers examples on various in situ characterization instrumental techniques Includes in-depth theoretical modeling utilizing advanced Density Functional Theory (DFT) methods

Heterogeneous Catalysis of Mixed Oxides - Makoto Misono
2013-02-28

The chemistry of metal oxides, both single and mixed metal oxides, relevant to heterogeneous catalysis such as relationships among the composition, structure, and chemical properties of mixed oxides, is provided in perspective. The important chemical properties in heterogeneous catalysis are acid-base and reduction-oxidation (redox) properties, where ionic radii, electronegativity, valency, and tendency to form covalent bond of constituent elements are most influential. Structural factors such as lattice defects and nonstoichiometry are also relevant. Although the surface of metal oxides is different from the solid bulk and changes depending on various factors, the surface reflects more or less the solid bulk and the knowledge of bulk properties is useful to understand the catalysis of mixed oxides. In some cases, the solid bulk actually takes part in catalysis. Other fundamental features of metal oxide catalysis like synergistic effects of more than two different active sites (acid and base, acid and oxidation, etc.) are also discussed.

Structure-activity and Selectivity Relationships in Heterogeneous Catalysis - 1991

Dynamics of Surfaces and Reaction Kinetics in Heterogeneous Catalysis - G.F. Froment 1997-09-03

Many processes of the chemical industry are based upon heterogeneous catalysis. Two important items of these processes are the development of the catalyst itself and the design and optimization of the reactor. Both aspects would benefit from rigorous and accurate kinetic modeling, based upon information on the working catalyst gained from classical steady state experimentation, but also from studies using surface science techniques, from quantum chemical calculations providing more insight into possible reaction pathways and from transient experimentation dealing with reactions and reactors. This information is seldom combined into a kinetic model and into a quantitative description of the process. Generally the catalytic aspects are dealt with by chemists and by physicists, while the chemical engineers are called upon for mechanical aspects of the reactor design and its control. The symposium "Dynamics of Surfaces and Reaction Kinetics in Heterogeneous Catalysis" aims at illustrating a more global and concerted approach through a number of prestigious keynote lectures and severely screened oral and poster presentations.

Catalysis - Sanjay K. Agarwal 1994

There is an increasing challenge for chemical industry and research institutions to find cost-efficient and environmentally sound methods of converting natural resources into fuels chemicals and energy. Catalysts are essential to these processes and the Catalysis Specialist Periodical Report series serves to highlight major developments in this area. This series provides systematic and detailed reviews of topics of interest to scientists and engineers in the catalysis field. The coverage includes all major areas of heterogeneous and homogeneous catalysis and also specific applications of catalysis such as NO_x control kinetics and experimental techniques such as microcalorimetry. Each chapter is compiled by recognised experts within their specialist fields and provides a summary of the current literature. This series will be of interest to all those in academia and industry who need an up-to-date critical analysis and summary of catalysis research and applications. Catalysis will be of

interest to anyone working in academia and industry that needs an up-to-date critical analysis and summary of catalysis research and applications. Specialist Periodical Reports provide systematic and detailed review coverage in major areas of chemical research. Compiled by teams of leading experts in their specialist fields, this series is designed to help the chemistry community keep current with the latest developments in their field. Each volume in the series is published either annually or biennially and is a superb reference point for researchers.

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Coal and Coal-Related Compounds - Toshiaki Kabe 2004-11-18

Coal is more abundant than petroleum and natural gas. Further, coal is not localized but can be used by many more countries than petroleum. Therefore, if we can establish coal utilization technology, coal will bring about a great contribution to human life and society. On the other hand, shortage of petroleum and natural gas are anticipated in the second half of the 21st century. To compensate, the use of coal is expected to gradually increase during the 21st century. In the future, the development of the coal utilization technology will become more and more important to insure the supply of liquid fuels for transportation and carbon sources for the manufacture of chemicals and plastic materials. In order to develop such technologies, the elucidation of the structure of coal is a fundamental area of study. Further, more efficient coal utilization technology must be established to meet environmental legislation. One of the key technologies for this purpose is catalysis. This volume provides detail of the basic and practical aspects of the science and technology of coal utilization with and without catalysts. The actual structure of coal, the chemistry included in the reactivity of coal, the methods to elucidate the structure of coal and re-action mechanisms of coal conversion, the most important catalyst for converting coal to liquid and gas, the role of the catalysts in coal conversion, the problems in the process engineering, and how to meet environmental regulations are discussed in detail. The recent progress in studies on the structure and reactivity of coal made over the last century is summarized and reviewed with emphasis on both fundamental and applied aspects of the science

and technology for coal processing in the presence and absence of catalysts. * This book highlights the issues faced in trying to discover more efficient coal utilization technology. * Provides detailed discussion on how to meet environmental regulations and legislation. * Fills the gap between both the scientific and practical sides of coal utilization with and without catalysts.

Structure-activity and Selectivity Relationships in Heterogeneous Catalysis - 1991

Heterogeneous Catalysis and Fine Chemicals IV - H.U. Blaser
1997-06-19

After three meetings in Poitiers, France, the 4th International Symposium on Heterogeneous Catalysis and Fine Chemicals was held under the auspices of the New Swiss Chemical Society in Basel, Switzerland. Fundamental as well as applied contributions on the use of heterogeneous catalysis for the preparation of fine chemicals were presented and discussed. The program consisted of 4 plenary lectures, 28 oral contributions and around 90 posters covering a broad range of reactions and catalytic aspects. 82 of these contributions are collected in the present proceedings, grouped into the following 8 topical areas: - Industrial and engineering problems (7 contributions) - Alkylation and acylation reactions (11 contributions) - Enantio- and diastereoselective hydrogenation reactions (9 contributions) - Chemoselective hydrogenation reactions (12 contributions) - Oxidation reactions (14 contributions) - Immobilized and encapsulated complex catalysts (12 contributions) - Zeolite and clay catalysts (12 contributions) - Miscellaneous topics (5 contributions)

Science and Technology in Catalysis - K Eguchi 2007-11-27

Unsteady-state operations of catalytic reactors provide plentiful opportunities for research and commercial realization of efficient heterogeneous catalytic processes. Forced unsteady state conditions generate unique distributions of process parameters and catalyst states often unattainable with traditional, steady-state operation. The unsteady-states can be created by periodic changes in input flow parameters, such

as changes in inlet temperature and composition, catalyst circulation through reaction and regeneration zones, or periodic flow reversals through fixed catalyst bed. This can result in increased productivity, selectivity, capital savings and operating cost reduction (higher energy efficiency). Efficient environmental technologies for treatment of toxic emissions, acid rain and greenhouse gas emissions can also be developed using the unsteady-state concept. The Proceedings communicate recent progress in these areas of research and promote future development. The aims are to establish relations between academia, industry, engineers and scientists from all over the world, to stimulate new catalytic technologies as well as fundamental research, and to create new concepts for the development of effective catalytic systems. It presents the most up-to-date research in catalysis. - contains the most recent developments in catalytic research - includes research finding as well as their application to industry - a thorough source of information on the latest developments of industrial catalysis in Japan

Elementary Reaction Steps in Heterogeneous Catalysis - R.W. Joyner
2012-12-06

This book comprises the proceedings of a NATO sponsored Advanced Research Workshop held from 1st November to 6th November 1992 in the delightful Chateau de Florans, Bedoin, Vaucluse, France and entitled 'Elementary Reaction Steps in Heterogeneous Catalysis.' The organisers are grateful to the Science Committee of NATO for their support of this meeting. This is believed to be the first wide ranging NATO ARW in the field of heterogeneous catalysis for 20 years, following a previous venture organised in Sardinia by Basolo and Burwell, of Northwestern University, Illinois, USA [1]. This volume collects the lecture presentations and reports on the lively Panel discussions. The idea for the meeting evolved from a series of International Symposia on Quantum Chemistry and Mechanism in Heterogeneous Catalysis. The first of these was held in Lyon, France in 1986, the second in Krakow, Poland in 1988 and the third in Berkeley, California in 1990. The organising committee of the present meeting was Bernard Bigot, France, Tony Farragher, Netherlands, Richard Joyner, UK, Mme. Danielle Olivier, France, and

Rutger van Santen, Netherlands, (Chairman). We wish to thank all members of the committee but in particular Bernard Bigot, who undertook the very extensive work involved in the local organisation with consummate skill and made our stay in Provence a great pleasure. Bernard Bigot's secretary, Mme. Marie-Noelle Coscat and Richard Joyner's secretary, Mrs. Pat Gibbs, also deserve our considerable thanks. There were fifty-four participants from eleven countries.

New Frontiers in Catalysis, Parts A-C - L. Guzzi 1993-04-20

These volumes comprise the proceedings of the major international meeting on catalysis which is held at 4 year intervals. The programme focussed on New Frontiers in Catalysis including nontraditional catalytic materials and environmental catalysis. The contributions cover a wide range of fundamental, applied, industrial and engineering aspects of catalysis. The extensive range of highly efficient industrial techniques for observing and characterizing catalytically important surfaces is evident. The programme covered the following sessions: Mechanism, theory, in situ methods; Catalytic reaction on atomically clean surfaces; Catalytic reaction on zeolites and related substances; New methods and principles for catalyst preparation; Hydrotreatment reactions (HDS, HDN); Characterization of catalysts, application of novel techniques; Selective oxidation; New catalytic aspects of heteropoly acids and related compounds; Reaction of hydrocarbons; Nontraditional catalytic materials; Fuel upgrading; Alkane activation; Acid-base catalysis; New selective catalytic reactions, fine chemicals; Environmental catalysis; Industrial catalysis, deactivation, reactivation; Synthesis from syngas; Electrocatalysis; Photocatalysis. The invited lectures and 433 papers included in these volumes present an update on all areas of catalysis and applications.

Catalysis: An Integrated Approach - B.A. Averill 1999-09-07

This book concentrates on industrially relevant reactions which are catalyzed by heterogeneous and homogeneous catalysts. Homogeneous catalysis by metal complexes is treated jointly with heterogeneous catalysis using metallic and non-metallic solids. In both areas the high degree of sophistication of spectroscopic techniques and theoretical

modelling has led to an enormous increase in our understanding at the molecular level. This holds for the kinetics of the reactions and the reactivities of the catalysts, as well as for the syntheses of the catalytic materials. The development of catalysis science since the first edition of this book has necessitated a thorough revision, including special chapters on biocatalysis, catalyst characterization and adsorption methods. The multidisciplinary nature of catalysis is reflected in the choice of a novel combination of basic disciplines which will be refreshing and inspiring to readers.

Scientific Bases for the Preparation of Heterogeneous Catalysts -

E. Gaigneaux 2002-08-29

It has become a tradition that every four years, the Université Catholique de Louvain and the Katholieke Universiteit Leuven jointly organize a symposium devoted to the scientific bases for the preparation of heterogeneous catalysts. These meetings bring together researchers from academia and industry and offer a forum for discussions on the chemistry involved in the preparation of industrial heterogeneous catalysts. This volume containing the Proceedings of the 8th International Symposium on Scientific Bases for the Preparation of Heterogeneous Catalysts consists of papers summarizing most of the 139 oral communications and posters selected by the international scientific committee, composed of 27 experts in the field of catalyst preparation, holding an industrial or academia appointment. The contributions focus on the aspects of catalyst preparation. The main topics are: new approaches in catalyst preparation; advanced preparations of nanoporous and mesoporous catalysts; catalysts preparation for special performances and purposes; catalysts for environmental purposes; and molecular catalysis. Emphasis is put on the role that catalysis can play as an essential element of sustainable development.

Equilibria and Dynamics of Gas Adsorption on Heterogeneous Solid Surfaces - W.A. Steele 1996-12-17

The fact that the surfaces of real solids are geometrically distorted and chemically non-uniform has long been realized by the scientists investigating various phenomena occurring on solid surfaces. Even in the

case when diffraction experiments show a well-organized bulk solid structure, the surface atoms or molecules will usually exhibit a much smaller degree of surface organization. In addition to the results obtained from electron diffraction, this can be seen in the impressive images obtained from STM and AFM microscopies. This geometric and chemical disorder is the source of the energetic heterogeneity for molecules adsorbing on real solid surfaces. Hundreds of papers have been published showing that this heterogeneity is a major factor in determining the behaviour of real adsorption systems. Studies of adsorption on energetically heterogeneous surfaces have proceeded along three somewhat separate paths, with only minor coupling of ideas. One was the study of adsorption equilibria on heterogeneous solid surfaces. The second path was the study of time evolution of adsorption processes such as surface diffusion or adsorption-desorption kinetics on heterogeneous surfaces, and the third was the study of adsorption in porous solids, or more generally, adsorption in systems with limited dimensions. The present monograph is a first attempt to provide a synthesis of the ways that surface geometric and energetic heterogeneities affect both the equilibria and the time evolution of adsorption on real solids. The book contains 17 chapters written by a team of internationally recognized specialists, some of whom have already published books on adsorption.

Zeolite Chemistry and Catalysis - L. Kubelková 1991-09-17

These proceedings reflect recent developments in the field of zeolite chemistry and catalysis with an emphasis on the role of a modifying component on the properties of the molecular sieve material. The plenary lectures and contributed papers concentrate on the problem of isomorphous substitution in a zeolitic framework; on the occlusion and the structure of metal, metal oxide, and metal sulphide clusters and complexes in the intracrystalline void volume of molecular sieves and zeolites as well as in the interlaminar space of layered compounds. Catalytic applications are discussed, not only in regard to traditional hydrocarbon transformation, but also in such areas as: reduction of SO₂, decomposition of NO, reactions of sulphur containing compounds and

conversion of CO, CO₂ to hydrocarbons or of alcohols to oxygenated products. Because the book provides valuable data and information on new achievements in the zeolite material science and application, it will be of considerable interest to all research groups involved in zeolite science.

Heterogeneous Catalysis and Fine Chemicals III - J. Barbier 1993-09-09

Heterogeneous catalysis plays a major role in the organic synthesis of specialty and fine chemicals. However, as the interaction between surface sites and functional groups is complex, more investigations are necessary into the effects of catalysts on the reaction mechanisms. The Third International Symposium on Heterogeneous Catalysis and Fine Chemicals provided an opportunity for discussions on the basic and practical aspects of this subject between researchers, manufacturers and users of solid catalysts for synthesis of fine chemicals. The present volume comprises the invited plenary lectures and research papers classified under the three main headings, hydrogenation, oxidation and acid-catalysis. All papers were refereed. A large variety of reactions are described, the emphasis being on selectivity, taking into account all aspects: chemo-, regio-, and stereoselectivity (including enantioselectivity) and on the change of these selectivities as a function of the characteristics of the catalysts and operating conditions.

Progress in Catalysis - K.J. Smith 1992-05-25

This volume contains papers and short communications presented at the 12th Canadian Symposium on Catalysis. The aim of the meeting was to present an update on new and established areas of catalysis research being performed in industry, government and university laboratories. Topics covered relate mainly to resource processing, such as heavy oil and natural gas upgrading, and to environmental issues. Approximately half the papers are included in sections on hydrogenation, carbon-carbon bond formation and environmental issues. The remaining papers cover general topics and homogeneous reactions. Examples include studies of hydroprocessing catalysts, carbon-carbon bond formation via methane oxidative coupling and dimerization of olefins, homogeneous catalysts in

polymerization and dimerization reactions, performance of pillared clays, metal-oxygen cluster compounds, zeolites and catalysts prepared by metal oxide vapour synthesis. Studies that address the environmental issues include wet-air oxidation, catalytic elimination of organics, oxidation reactions and catalyst regeneration. The book provides practitioners of catalysis with an update on a wide number of topics and

will be particularly useful to those interested in an overview of current catalysis research activities. Specialists in the areas of hydrogenation, carbon-carbon bond formation, homogeneous catalysis and environmental issues will also find a valuable set of new data and interesting discussions on these topics.

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