Electrocatalysis Theoretical Foundations And Model Experiments Volume 14 Advances In Electrochemical Sciences And Engineering

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Carbon-Based Metal-Free Catalysts

A profound understanding of the physical laws underlying energy converters is a prerequisite for a sustainable use of our energy resources. The aim of this textbook is to provide a unified view on the different energy conversion processes ranging from power plants to solar cells. It offers an interdisciplinary introduction to energy sciences for senior undergraduate and graduate students from natural sciences and engineering. The central theme is the treatment of energy converters as open thermodynamical systems and the performance of efficiency analyses, based on the concept of exergy. Presents the physics behind the most important energy converters in a unified framework. Evaluates the performance of ideal and realistic energy converters in terms of energy and exergy efficiencies Provides basic concepts needed for a discussion of energy converters, such as chemical and applied thermodynamics, electrochemistry and solid state physics. About the Authors Katharina Krischer is aprofessor of physics at the Technische Universität München, Germany. She has taught lectures on energy sciences for undergraduate and graduate students for more than 10 years. Her research topics include the photo-electrochemical production of solar fuels. Konrad Schönleber is a researcher in the group of Prof. Krischer which he joined after graduating in physics from the Technische Universität München. His research interest focuses on light-driven semiconductor electrochemistry and its application for renewable energies.

Advanced Catalytic Materials

Electrochemical Power Sources

This book addresses some essential topics in the science of energy converting devices emphasizing recent aspects of nano-derived materials in the application for the protection of the environment, storage, and energy conversion. The aim, therefore, is to provide the basic background knowledge. The electron transfer process and structure of the electric double layer and the interaction of species with surfaces and the interaction, reinforced by DFT theory for the current and incoming generation of fuel cell scientists to study the interaction of the catalytic centers with their supports. The chief focus of the chapters is on materials based on precious and non-precious centers for the hydrogen electrode, the oxygen electrode, energy storage, and in remediation applications, where the common issue is the rate-determining step in multi-electron charge transfer processes in electrocatalysis. These approaches are used in a large extent in science and technology, so that each chapter demonstrates the connection of electrochemistry, in addition to chemistry, with different areas, namely, surface science, biochemistry, chemical engineering, and chemical physics.

Density Functional Theory

Catalysis in Electrochemistry: From Fundamental Aspects to Strategies for Fuel Cell Development is a modern, comprehensive reference work on catalysis in electrochemistry, including principles, methods, strategies, and applications. It points out differences between catalysis at gas/surfaces and electrochemical interfaces, along with the future possibilities and impact of electrochemical science on energy problems. This book contributes both to fundamental science; experience in the design, preparation, and characterization of electrocatalytic materials; and the industrial application of electrocatalytic materials for electrochemical reactions. This is an essential resource for scientists globally in academia, industry, and government institutions.

Fundamentals of Electrocatalyst Materials and Interfacial Characterization

Metal Oxide-Based Nanostructured Electrocatalysts for Fuel Cells, Electrolyzers, and Metal-Air Batteries is a comprehensive book summarizing the recent overview of these new materials developed to date. The book is motivated by research that focuses on the reduction of noble metal content in catalysts to reduce the cost associated to the entire system. Metal oxides gained significant interest in heterogeneous catalysis for basic research and industrial deployment. Metal Oxide-Based Nanostructured Electrocatalysts for Fuel Cells, Electrolyzers, and Metal-Air Batteries puts these opportunities and

challenges into a broad context, discusses the recent researches and technological advances, and finally provides several pathways and guidelines that could inspire the development of ground-breaking electrochemical devices for energy production or storage. Its primary focus is how materials development is an important approach to produce electricity for key applications such as automotive and industrial. The book is appropriate for those working in academia and R&D in the disciplines of materials science, chemistry, electrochemistry, and engineering. Includes key aspects of materials design to improve the performance of electrode materials for energy conversion and storage device applications Reviews emerging metal oxide materials for hydrogen production, hydrogen oxidation, oxygen reduction and oxygen evolution Discusses metal oxide electrocatalysts for water-splitting, metal-air batteries, electrolyzer, and fuel cell applications

Vibrational Spectroscopy at Electrified Interfaces

Reviews the latest theory, techniques, and applications Surface vibrational spectroscopy techniques probe the structure and composition of interfaces at the molecular level. Their versatility, coupled with their non-destructive nature, enables in-situ measurements of operating devices and the monitoring of interface-controlled processes under reactive conditions. Vibrational Spectroscopy at Electrified Interfaces explores new and emerging applications of Raman, infrared, and non-linear optical spectroscopy for the study of charged interfaces. The book draws from hundreds of findings reported in the literature over the past decade. It features an internationally respected team of authors and editors, all experts in the field of vibrational spectroscopy at surfaces and interfaces. Content is divided into three parts: Part One, Nonlinear Vibrational Spectroscopy, explores properties of interfacial water, ions, and biomolecules at charged dielectric, metal oxide, and electronically conductive metal catalyst surfaces. In addition to offering plenty of practical examples, the chapters present the latest measurement and instrumental techniques. Part Two, Raman Spectroscopy, sets forth highly sensitive approaches for the detection of biomolecules at solid-liquid interfaces as well as the use of photon depolarization strategies to elucidate molecular orientation at surfaces. Part Three, IRRAS Spectroscopy (including PM-IRRAS), reports on wide-ranging systems—from small fuel molecules at well-defined surfaces to macromolecular complexes—that serve as the building blocks for functional interfaces in devices designed for chemical sensing and electric power generation. The Wiley Series on Electrocatalysis and Electrochemistry is dedicated to reviewing important advances in the field, exploring how these advances affect industry. The series defines what we currently know and can do with our knowledge of electrocatalysis and electrochemistry as well as forecasts where we can expect the field to be in the future.

Modeling and Simulation of Heterogeneous Catalytic Reactions

The Handbook of Materials Modeling, 2nd edition is a six-volume major reference serving a steadily growing community at the intersection of two mainstreams of global research: computational science and materials science and technology. This

extensively expanded new edition reflects the significant developments in all aspects of computational materials research over the past decade, featuring progress in simulations at multiple scales and increasingly more realistic materials models. Thematically separated into two mutually dependent sets – “Methods: Theory and Modeling (MTM)” and “Applications: Current and Emerging Materials (ACE)” – the handbook runs the entire gamut from theory and methods to simulations and applications. Readers benefit from its in-depth coverage of a broad methodological spectrum extending from advanced atomistic simulations of rare events to data-driven artificial intelligence strategies for materials informatics in the set MTM, as well as forefront emphasis on materials of far-ranging societal importance such as photovoltaics and energy-relevant oxides, and cutting-edge applications to materials for spintronic devices, graphene, cement, and glasses in the set ACE. The thorough, interconnected coverage of methods and applications, together with a line-up of internationally acclaimed editors and authors, will ensure the Handbook of Material Modeling’s standing as an enduring source of learning and inspiration for a global community of computational materials scientists.

Surface Science

The book starts with a theoretical understanding of electrocatalysis in the framework of density functional theory followed by a vivid review of oxygen reduction reactions. A special emphasis has been placed on electrocatalysts for a proton-exchange membrane-based fuel cell where graphene with noble metal dispersion plays a significant role in electron transfer at thermodynamically favourable conditions. The latter part of the book deals with two 2D materials with high economic viability and process ability and MoS2 and WS2 for their prospects in water-splitting from renewable energy.

Metal Oxide-Based Nanostructured Electrocatalysts for Fuel Cells, Electrolyzers, and Metal-Air Batteries

The Nobel Prize in Chemistry 2007 awarded to Gerhard Ertl for his groundbreaking studies in surface chemistry highlighted the importance of heterogeneous catalysis not only for modern chemical industry but also for environmental protection. Heterogeneous catalysis is seen as one of the key technologies which could solve the challenges associated with the increasing diversification of raw materials and energy sources. It is the decisive step in most chemical industry processes, a major method of reducing pollutant emissions from mobile sources and is present in fuel cells to produce electricity. The increasing power of computers over the last decades has led to modeling and numerical simulation becoming valuable tools in heterogeneous catalysis. This book covers many aspects, from the state-of-the-art in modeling and simulations of heterogeneous catalytic reactions on a molecular level to heterogeneous catalytic reactions from an engineering perspective. This first book on the topic conveys expert knowledge from surface science to both chemists and engineers interested in heterogeneous catalysis. The well-known and international authors comprehensively present many aspects of

the wide bridge between surface science and catalytic technologies, including DFT calculations, reaction dynamics on surfaces, Monte Carlo simulations, heterogeneous reaction rates, reactions in porous media, electro-catalytic reactions, technical reactors, and perspectives of chemical and automobile industry on modeling heterogeneous catalysis. The result is a one-stop reference for theoretical and physical chemists, catalysis researchers, materials scientists, chemical engineers, and chemists in industry who would like to broaden their horizon and get a substantial overview on the different aspects of modeling and simulation of heterogeneous catalytic reactions.

Electrocatalysts for Fuel Cells and Hydrogen Evolution

Electrochemical Power Sources (EPS) provides in a concise way the operational features, major types, and applications of batteries, fuel cells, and supercapacitors • Details the design, operational features, and applications of batteries, fuel cells, and supercapacitors • Covers improvements of existing EPSs and the development of new kinds of EPS as the results of intense R&D work • Provides outlook for future trends in fuel cells and batteries • Covers the most typical battery types, fuel cells and supercapacitors; such as zinc-carbon batteries, alkaline manganese dioxide batteries, mercury-zinc cells, lead-acid batteries, cadmium storage batteries, silver-zinc batteries and modern lithium batteries

Electrocatalysis

This book explores key parameters, properties and fundamental concepts of electrocatalysis. It also discusses the engineering strategies, current applications in fuel-cells, water-splitting, metal-ion batteries, and fuel generation. This book elucidates entire category viewpoints together with industrial applications. Therefore, all the sections of this book emphasize the recent advances of different types of electrocatalysts, current challenges, and state-of-the-art studies through detailed reviews. This book is the result of commitments by numerous experts in the field from various backgrounds and expertise and appeals to industrialists, researchers, scientists and in addition understudies from various teaches.

Physics of Energy Conversion

This book is based on a graduate course and suitable as a primerfor any newcomer to the field, this book is a detailed introductionto the experimental and computational methods that are used tostudy how solid surfaces act as catalysts. Features include: First comprehensive description of modern theory ofheterogeneous catalysis Basis for understanding and designing experiments in the field Allows reader to understand catalyst design principles Introduction to important elements of energy transformationtechnology Test driven at Stanford University over several semesters

Electrogenerative Oxidation of Model Alcohols with Packed Bed Electrocatalysts

Power Ultrasound in Electrochemistry

Written by an excellent, highly experienced and motivated team of lecturers, this textbook is based on one of the most successful courses in catalysis and as such is tried-and-tested by generations of graduate and PhD students, i.e. the Catalysis-An-Integrated-Approach (CAIA) course organized by NIOK, the Dutch Catalysis research school. It covers all essential aspects of this important topic, including homogeneous, heterogeneous and biocatalysis, but also kinetics, catalyst characterization and preparation, reactor design and engineering. The perfect source of information for graduate and PhD students in chemistry and chemical engineering, as well as for scientists wanting to refresh their knowledge

Advances In Hydrogen Generation Technologies

Surface chemistry is an essential and developing area of physical chemistry and one that has become increasingly interdisciplinary. The Second Edition of Surface Science: Foundations of Catalysis and Nanoscience has been fully revised and updated to reflect all the latest developments in the field and now includes an extensive discussion about nanoparticle growth and the quantum confinement effects in nanoscale systems. Two new chapters have been added and discuss The Liquid/Solid Interface and Non-Thermal Reactions, and Photon and Electron Stimulated Chemistry and Atom Manipulation. There are now many more worked examples included throughout to help students develop their problem-solving skills.

Fundamental Concepts in Heterogeneous Catalysis

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.

Interfacial Electrochemistry

Electrochemical Processes in Biological Systems

Todays chemical industry processes worldwide largely depend on catalytic reactions and the desirable future evolution of this industry toward more selective products, more environmentally friendly products, more energy-efficient processes, a smaller use of hazardous reagents, and a better use of raw materials also largely involves the development of better catalysts and, specifically, purposely designed catalytic materials. The careful study and development of the new-generation catalysts involve relatively large groups of specialists in universities, research centers, and industries, joining forces from different scientific and technical disciplines. This book has put together recent, state-of-the-art topics on current trends in catalytic materials and consists of 16 chapters.

Catalysis

The book provides a systematic and profound account of scientific challenges in fuel cell research. The introductory chapters bring readers up to date on the urgency and implications of the global energy challenge, the prospects of electrochemical energy conversion technologies, and the thermodynamic and electrochemical principles underlying the operation of polymer electrolyte fuel cells. The book then presents the scientific challenges in fuel cell research as a systematic account of distinct components, length scales, physicochemical processes, and scientific disciplines. The main part of the book focuses on theory and modeling. Theoretical tools and approaches, applied to fuel cell research, are presented in a self-contained manner. Chapters are arranged by different fuel cell materials and components, and sections advance through the hierarchy of scales, starting from molecular-level processes in proton-conducting media or electrocatalytic systems and ending with performance issues at the device level, including electrochemical performance, water management, durability, and analysis of failure mechanisms. Throughout, the book gives numerous examples of formidable scientific challenges as well as of tools to facilitate materials design and development of diagnostic methods. It reveals reserves for performance improvements and uncovers misapprehensions in scientific understanding that have misled or may continue to mislead technological development. An indispensable resource for scientifically minded and practically oriented researchers, this book helps industry leaders to appreciate the contributions of fundamental research, and leaders of fundamental research to appreciate the needs of industry.

Catalysis: An Integrated Approach

Catalysis has revolutionized the chemical industry as catalysts are used in the production of most chemicals, resulting in a multi-billion euro business. This advanced textbook is a must-have for all Master and PhD students in the field as it adopts a

unique interdisciplinary approach to the topic of catalysis. It presents a collection of chapters that explain the fundamentals of catalysis as the area has developed over the past decades and introduces new catalytic systems that are of becoming of increasing current importance. It covers all the essential principles, ranging from catalytic processes at the molecular level to catalytic reactor design and includes several case studies illustrating the importance of catalysts in the chemical industry.

Graphene Chemistry

This proceedings volume comprises the invited plenary lectures, contributed and poster papers presented at a symposium organised to mark the successful inauguration of the world's first commercial plant for production of gasoline from natural gas, based on the Mobil methanol-to-gasoline process. The objectives of the Symposium were to present both fundamental research and engineering aspects of the development and commercialization of gas-to-gasoline processes. These include steam reforming, methanol synthesis and methanol-to-gasoline. Possible alternative processes e.g. MOGD, Fischer-Tropsch synthesis of hydrocarbons, and the direct conversion of methane to higher hydrocarbons were also considered. The papers in this volume provide a valuable and extremely wide-ranging overview of current research into the various options for natural gas conversion, giving a detailed description of the gas-to-gasoline process and plant. Together, they represent a unique combination of fundamental surface chemistry catalyst characterization, reaction chemistry and engineering scale-up and commercialization.

Choice

Springer Handbook of Electrochemical Energy

Wiley Series on Electrocatalysis and Electrochemistry Fuel Cell Catalysis A Surface Science Approach A Core reference on fuel cell catalysis Fuel cells represent an important alternative energy source and a very active area of research. Fuel Cell Catalysis brings together world leaders in this field, providing a unique combination of state-of-the-art theory and computational and experimental methods. With an emphasis on understanding fuel cell catalysis at the molecular level, this text covers fundamental principles, future challenges, and important current research themes. Fuel Cell Catalysis: Provides a molecular-level description of catalysis for low-temperature polymer-electrolyte membrane fuel cells, including both hydrogen-oxygen cells and direct alcohol cells Examines catalysis issues of both anode and cathode such as oxygen reduction, alcohol oxidation, and CO tolerance Features a timely and forward-looking approach through emphasis on novel aspects such as computation and bio-inspiration Reviews the use and potential of surface-sensitive techniques like

vibrational spectroscopy (IR, Raman, nonlinear spectroscopy, laser), scanning tunneling microscopy, X-ray scattering, NMR, electrochemical techniques, and more Reviews the use and potential of such modern computational techniques as DFT, ab initio MD, kinetic Monte Carlo simulations, and more Surveys important trends in reactivity and structure sensitivity, nanoparticles, "dynamic" catalysis, electrocatalysis vs. gas-phase catalysis, new experimental techniques, and nontraditional catalysts This cutting-edge collection offers a core reference for electrochemists, electrocatalysis researchers, surface and physical chemists, chemical and automotive engineers, and researchers in academia, research institutes, and industry.

Electrocatalysis on non-metallic surfaces

This book presents both the fundamentals concepts and latestachievements of a field that is growing in importance since itrepresents a possible solution for global energy problems. It focuses on an atomic-level understanding ofheterogeneous catalysis involved in important energy conversionprocesses. It presents a concise picture for the entire areaof heterogeneous catalysis with vision at the atomic- and nano-scales, from synthesis, ex-situ and in-situ characterization,catalytic activity and selectivity, to mechanistic understandingbased on experimental exploration and theoretical simulation. The book: Addresses heterogeneous catalysis, one of the crucialtechnologies employed within the chemical and energyindustries Presents the recent advances in the synthesis andcharacterization of nanocatalysts as well as a mechanisticunderstanding of catalysis at atomic level for important processesof energy conversion Provides a foundation for the potential design ofrevolutionarily new technical catalysts and thus the furtherdevelopment of efficient technologies for the global energyeconomy Includes both theoretical studies and experimentalexploration Is useful as both a textbook for graduate and undergraduatestudents and a reference book for scientists and engineers inchemistry, materials science, and chemical engineering

Catalysis

Among energy sources, hydrogen gas is clean and renewable and has the potential to solve the growing energy crisis in today's society because of its high-energy density and noncarbon fuel properties. It is also used for many potential applications in nonpolluting vehicles, fuel cells, home heating systems, and aircraft. In addition, using hydrogen as an energy carrier is a long-term option to reduce carbon dioxide emissions worldwide by obtaining high-value hydrocarbons through the hydrogenation of carbon dioxide. This book presents the recent progresses and developments in water-splitting processes as well as other hydrogen generation technologies with challenges and future perspectives from the point of energy sustainability.

Chemical Process Design and Simulation: Aspen Plus and Aspen Hysys Applications

A rigorous outline of the basic concepts (phenomena, processes, laws) forming the subject matter of modern theoretical and applied electrochemistry, originally published in Russian in 1988 by Khimiya Press, Moscow. In the present English edition three supplementary chapters have been added, on photo

Catalysis in Electrochemistry

Offering comprehensive coverage of this hot topic, this two-volume handbook and ready reference treats a wide range of important aspects, from synthesis and catalytic properties of carbon materials to their applications as metal-free catalysts in various important reactions and industrial processes. Following a look at recent advances in the development of carbon materials as carbon-based metal-free catalysts, subsequent sections deal with a mechanistic understanding for the molecular design of efficient carbon-based metal-free catalysts, with a special emphasis on heteroatom-doped carbon nanotubes, graphene, and graphite. Examples of important catalytic processes covered include clean energy conversion and storage, environmental protection, and synthetic chemistry. With contributions from world-leading scientists, this is an indispensable source of information for academic and industrial researchers in catalysis, green chemistry, electrochemistry, materials science, nanotechnology, energy technology, and chemical engineering, as well as graduates and scientists entering the field.

Fuel Cell Catalysis

Electrochemistry is an old branch of physical chemistry. Due to the development of surface sensitive techniques, and a technological interest in fuel cells and batteries, it has recently undergone a rapid development. This textbook treats the field from a modern, atomistic point of view while integrating the older, macroscopic concepts. The increasing role of theory is reflected in the presentation of the basic ideas in a way that should appeal to experimentalists and theorists alike. Special care is taken to make the subject comprehensible to scientists from neighboring disciplines, especially from surface science. The book is suitable for an advanced course at the master or Ph.D. level, but should also be useful for practicing electrochemists, as well as to any scientist who wants to understand modern electrochemistry.

Handbook of Materials Modeling

This comprehensive handbook covers all fundamentals of electrochemistry for contemporary applications. It provides a rich presentation of related topics of electrochemistry with a clear focus on energy technologies. It covers all aspects of

electrochemistry starting with theoretical concepts and basic laws of thermodynamics, non-equilibrium thermodynamics and multiscale modeling. It further gathers the basic experimental methods such as potentiometry, reference electrodes, ion-sensitive electrodes, voltammetry and amperometry. The contents cover subjects related to mass transport, the electric double layer, ohmic losses and experimentation affecting electrochemical reactions. These aspects of electrochemistry are especially examined in view of specific energy technologies including batteries, polymer electrolyte and biological fuel cells, electrochemical capacitors, electrochemical hydrogen production and photoelectrochemistry. Organized in six parts, the overall complexity of electrochemistry is presented and makes this handbook an authoritative reference and definitive source for advanced students, professionals and scientists particularly interested in industrial and energy applications.

Fundamentals of Electrochemistry

What are the chemical aspects of graphene as a novel 2D material and how do they relate to the molecular structure? This book addresses these important questions from a theoretical and computational standpoint. Graphene Chemistry: Theoretical Perspectives presents recent exciting developments to correlate graphene's properties and functions to its structure through state-of-the-art computational studies. This book focuses on the chemistry aspect of the structure-property relationship for many fascinating derivatives of graphene; various properties such as electronic structure, magnetism, and chemical reactivity, as well as potential applications in energy storage, catalysis, and nanoelectronics are covered. The book also includes two chapters with significant experimental portions, demonstrating how deep insights can be obtained by joint experimental and theoretical efforts. Topics covered include: Graphene ribbons: Edges, magnetism, preparation from unzipping, and electronic transport Nanographenes: Properties, reactivity, and synthesis Clar sextet rule in nanographene and graphene nanoribbons Porous graphene, nanomeshes, and graphene-based architecture and assemblies Doped graphene: Theory, synthesis, characterization and applications Mechanisms of graphene growth in chemical vapor deposition Surface adsorption and functionalization of graphene Conversion between graphene and graphene oxide Applications in gas separation, hydrogen storage, and catalysis Graphene Chemistry: Theoretical Perspectives provides a useful overview for computational and theoretical chemists who are active in this field and those who have not studied graphene before. It is also a valuable resource for experimentalist scientists working on graphene and related materials, who will benefit from many concepts and properties discussed here.

Methane Conversion

This unique discussion meeting will bring electrochemists, surface scientists and theoreticians together and foster the development of both in situ spectroscopic methods in electrochemistry and theoretical methods which model the electrocatalytic interface. This unique discussion meeting will bring electrochemists, surface scientists and theoreticians

together and foster the development of both in situ spectroscopic methods in electrochemistry and theoretical methods which model the electrocatalytic interface. It will be opened with an introductory lecture by Marc Koper from Leiden University in the Netherlands. Discussion sessions: Structure in Electrocatalysis: from nanoparticles to single crystals Spectroscopy and Electrocatalysis Hydrogen oxidation and oxygen reduction Biological electrocatalysis and alcohols as fuels

Heterogeneous Catalysis at Nanoscale for Energy Applications

The use of power ultrasound to promote industrial electrochemical processes, or sonoelectrochemistry, was first discovered over 70 years ago, but recently there has been a revived interest in this field. Sonoelectrochemistry is a technology that is safe, cost-effective, environmentally friendly and energy efficient compared to other conventional methods. The book contains chapters on the following topics, contributed from leading researchers in academia and industry: Use of electrochemistry as a tool to investigate Cavitation Bubble Dynamics Sonoelectroanalysis Sonoelectrochemistry in environmental applications Organic Sonoelectrosynthesis Sonoelectrodeposition Influence of ultrasound on corrosion kinetics and its application to corrosion tests Sonoelectropolymerisation Sonoelectrochemical production of nanomaterials Sonochemistry and Sonoelectrochemistry in hydrogen and fuel cell technologies

Oxygen Reduction Reactions

New Frontiers in Nanochemistry: Concepts, Theories, and Trends, Volume 1: Structural Nanochemistry is the first volume of the new three-volume set that explains and explores the important concepts from various areas within the nanosciences. This first volume focuses on structural nanochemistry and encompasses the general fundamental aspects of nanochemistry while simultaneously incorporating crucial material from other fields, in particular mathematic and natural sciences, with specific attention to multidisciplinary chemistry. Under the broad expertise of the editor, the volume contains 50 concise yet comprehensive entries from world-renowned scholars, alphabetically organizing a multitude of essential basic and advanced concepts, ranging from algebraic chemistry to new energy technology, from the bondonic theory of chemistry to spintronics, and from fractal dimension and kinetics to quantum dots and tight binding—and much more. The entries contain definitions, short characterizations, uses and usefulness, limitations, references, and more.

Theory and Experiment in Electrocatalysis

New Frontiers in Nanochemistry: Concepts, Theories, and Trends

Electrocatalysis

Catalysts speed up a chemical reaction or allow for reactions to take place that would not otherwise occur. The chemical nature of a catalyst and its structure are crucial for interactions with reaction intermediates. An electrocatalyst is used in an electrochemical reaction, for example in a fuel cell to produce electricity. In this case, reaction rates are also dependent on the electrode potential and the structure of the electrical double-layer. This work provides a valuable overview of this rapidly developing field by focusing on the aspects that drive the research of today and tomorrow. Key topics are discussed by leading experts, making this book a must-have for many scientists of the fi eld with backgrounds in different disciplines, including chemistry, physics, biochemistry, engineering as well as surface and materials science. This book is volume XIV in the series "Advances in Electrochemical Sciences and Engineering".

Methods for Electrocatalysis

A comprehensive and example oriented text for the study of chemical process design and simulation Chemical Process Design and Simulation is an accessible guide that offers information on the most important principles of chemical engineering design and includes illustrative examples of their application that uses simulation software. A comprehensive and practical resource, the text uses both Aspen Plus and Aspen Hysys simulation software. The author describes the basic methodologies for computer aided design and offers a description of the basic steps of process simulation in Aspen Plus and Aspen Hysys. The text reviews the design and simulation of individual simple unit operations that includes a mathematical model of each unit operation such as reactors, separators, and heat exchangers. The author also explores the design of new plants and simulation of existing plants where conventional chemicals and material mixtures with measurable compositions are used. In addition, to aid in comprehension, solutions to examples of real problems are included. The final section covers plant design and simulation of processes using nonconventional components. This important resource: Includes information on the application of both the Aspen Plus and Aspen Hysys software that enables a comparison of the two software systems Combines the basic theoretical principles of chemical process and design with real-world examples Covers both processes with conventional organic chemicals and processes with more complex materials such as solids, oil blends, polymers and electrolytes Presents examples that are solved using a new version of Aspen software, ASPEN One 9 Written for students and academics in the field of process design, Chemical Process Design and Simulation is a practical and accessible guide to the chemical process design and simulation using proven software.

Russian Journal of Electrochemistry

Polymer Electrolyte Fuel Cells

Demonstrates how anyone in math, science, and engineering canmaster DFT calculations Density functional theory (DFT) is one of the most frequentlyused computational tools for studying and predicting the propertiesof isolated molecules, bulk solids, and material interfaces,including surfaces. Although the theoretical underpinnings of DFTare quite complicated, this book demonstrates that the basicconcepts underlying the calculations are simple enough to beunderstood by anyone with a background in chemistry, physics,engineering, or mathematics. The authors show how the widespreadavailability of powerful DFT codes makes it possible for studentsand researchers to apply this important computational technique toa broad range of fundamental and applied problems. Density Functional Theory: A Practical Introductionoffers a concise, easy-to-follow introduction to the key conceptsand practical applications of DFT, focusing on plane-wave DFT. Theauthors have many years of experience introducing DFT to studentsfrom a variety of backgrounds. The book therefore offers severalfeatures that have proven to be helpful in enabling students tomaster the subject, including: Problem sets in each chapter that give readers the opportunityto test their knowledge by performing their own calculations Worked examples that demonstrate how DFT calculations are usedto solve real-world problems Further readings listed in each chapter enabling readers toinvestigate specific topics in greater depth This text is written at a level suitable for individuals from avariety of scientific, mathematical, and engineering backgrounds.No previous experience working with DFT calculations is needed.

Industrial Catalysis

Now in it's 3rd Edition, Industrial Catalysis offers all relevant information on catalytic processes in industry, including many recent examples. Perfectly suited for self-study, it is the ideal companion for scientists who want to get into the field or refresh existing knowledge. The updated edition covers the full range of industrial aspects, from catalyst development and testing to process examples and catalyst recycling. The book is characterized by its practical relevance, expressed by a selection of over 40 examples of catalytic processes in industry. In addition, new chapters on catalytic processes with renewable materials and polymerization catalysis have been included. Existing chapters have been carefully revised and supported by new subchapters, for example, on metathesis reactions, refinery processes, petrochemistry and new reactor concepts. "I found the book accesible, readable and interesting - both as a refresher and as an introduction to new topics - and a convenient first reference on current industrial catalytic practise and processes." Excerpt from a book review for the second edition by P. C. H. Mitchell, Applied Organometallic Chemistry (2007)