Heterogeneous Catalysis For Todays Challenges Synthesis Characterization And Applications Rsc Green Chemistry

There is a growing interest in the development of sustainable processes for the synthesis of pharmaceuticals and this book bridges the divide between industrial examples and the fundamental chemistry. It explains the basic principles of using transition metal catalysis with several green approaches for the synthesis of pharmaceuticals. The topic is an important one for green chemistry and the chapters in this book on hydroformylation, green oxidation and olefin metathesis will also be of interest to both medicinal and organic chemists. Written by leading experts in the field, it provides a valuable and easy tool for scientists and industrialists who require information regarding this topic.

Almost two centuries after the word "catalysis" was first introduced by Berzelius in 1835, the field has been developed to the point where heterogeneous catalysis is at the heart of our today's chemical industry. Nevertheless, one of the grand challenges in this area is being able to tune and design efficient catalysts for processes of interest. In order to do so, a molecular-level understanding of heterogeneous catalysts is of the utmost importance and indeed is a primary focus of modern catalysis research. Conventionally, the single most thermodynamically stable structure of the catalyst obtained under the reaction conditions had been considered as the reactive structure. However, catalysts in the subnano regime, in which there are only up to around 30 atoms per cluster, undergo structural dynamics under reaction conditions, which is triggered by high temperatures and pressures, and changing adsorbates. Using density functional theory and global optimization for structure prediction, in combination with statistical mechanics, we have recently shown that this dynamic fluxionality causes supported clusters to populate numerous distinct structural states under catalytic conditions. Furthermore, considering the single most stable structure gives unrealistic picture and inconsistent results with experiments. Therefore, the catalyst structure should be viewed as an evolving statistical ensemble of many structures. This new idea reforms the accepted models and calls for a new theory and modeling approaches leading to revised design strategies. Our ensemble-average model along with careful sampling of relevant structures suggest that many earlier studies might have overlooked the actual active sites. Ensemble phenomena lead to surprising exceptions from established rules of catalysis such as scaling relations. Catalyst deactivation (sintering, poisoning) is also an ensemble property, and its extent of mitigation can be predicted through the new paradigm. For example, in collaboration with Scott Anderson (U. Utah), we showed that nano-alloying with Sn suppresses both sintering and coking of Pt clusters deposited on SiO2, and on Al2O3, in conditions of thermal dehydrogenation. Theoretically, we showed that this is an ensemble effect, whereby adding Sn quenches electronic spin in all thermally accessible Ptn isomers clusters, closing most of the reaction paths toward deeper dehydrogenation. The ensemble approach leads to a different view on the reaction kinetics and thermodynamics. Chemically distinct states of the catalyst get populated as T increases, and if these states have barriers significantly different from that of the global minimum the Arrhenius plot should be nonlinear. Therefore, we proposed a modification to the Arrhenius equation using an ensemble-average representation. Spectral signatures are also no longer those of a single structure. In this regard, we showed that for highly fluxional supported nanoclusters, the customary extraction of the oxidation state of the metal from X-ray Absorption Near Edge Structure (XANES) data by fitting to the bulk standards has to be revised. Fitting the experimental spectrum to the calculated spectra of computed ensembles of supported clusters can in contrast provide good agreement and insight on the spectrum-composition- structure relation. These findings were enabled by advances in theory, such as global optimization and subsequent utilization of multiple local minima and pathways sampling as well as catalyst characterization under working condition. More importantly, our proposed model has been tested and confirmed by several experiments, as shown in joint publications with the experimental groups.

Many modern surface coatings and adhesives are derived from fossil feedstocks. With fossil fuels becoming more polluting and expensive to extract as supplies dwindle, industry is turning increasingly to nature, mimicking natural solutions using renewable raw materials and employing new technologies. Highlighting sustainable technologies and applications of renewable raw materials within the framework of green and sustainable chemistry, circular economy and resource efficiency, this book provides a cradle-to-cradle perspective. From potential feedstocks to recycling/reuse opportunities and the de-manufacture of adhesives and solvents, green chemistry principles are applied to all aspects of surface coating, printing, adhesive and sealant manufacture. This book is ideal for students, researchers and industrialists working in green sustainable chemistry, industrial coatings, adhesives, inks and printing technologies.

Catalysis is a fundamentally sustainable process which can be used to produce a wide range of chemicals and their intermediates. Focussing on those catalytic processes which offer the most sustainability, this two-part book explores recent developments in this field, as well as examining future challenges. Focussing on catalysis through non-endangered metals, chapters are dedicated to the most important sustainable metals in catalysis: titanium, iron and aluminium. Remaining chapters examine several other important metals. Green aspects of the various reactions are also discussed, such as atom economy and use of green solvents and other reaction conditions. Together with “Sustainable Catalysis: Without Metals or Other Endangered Elements”, these books examine the progress in sustainable catalysis in all areas of chemistry, and are an important reference for researchers working in catalysis and green chemistry.

What does cotton candy, which dissolves at the touch, have in common with Kevlar, used for bullet-proof vests? How can our understanding of such materials help us to tackle essential problems of the 21st century? Materials play a key role in our search for solutions to many pressing issues. They underpin many industries, are critical for the development of consumer goods, are essential components of medical diagnostic techniques, offer hope for the treatment of currently incurable diseases, and provide answers to environmental problems. This handbook is a guide to the materials we rely on for the future. Materials for the 21st Century serves as a useful resource for undergraduate and high school students preparing for a career in physical sciences, life sciences,or engineering, by helping them to identify new areas of interest. It is also an excellent reference for readers interested in learning more about the diverse range of materials that underlie key aspects of our economy and everyday lives.

This book aims to provide an overview of the design, limitations and challenges of heterogeneous catalysts for energy applications.

Aerogels have been in use for over 80 years and have been utilised in a wide variety of applications, in particular, there has been growing use of insulating nanoporous materials in the aerospace industry. Recent awareness of the environmental implications of materials has driven researchers to develop new green materials, with aerogels being developed using biobased constituents, such as polysaccharides and proteins. Recently, biobased components, such as cellulose nanocrystals, have replaced synthetic counterparts in the production of nanoporous materials. Biobased Aerogelsis the first book to cover aerogel research from a green perspective, using commentary and analysis from leading researchers working in the field. Aerogels based on polysaccharides and proteins, their preparation and characterisation will be covered in detail, with further discussion highlighting properties such as surface morphology, shape recovery, mechanical properties and adsorption capacity. This insightful and timely publication will provide essential reading for those researchers and industrialists working within the green chemistry field.

Polymer science faces the challenge of meeting growing market demand for polymers whilst achieving sustainability through environmentally friendly processes. Microwave heating has emerged as a greener technique that accelerates a variety of chemical reactions, including polymerization. Microwave-assisted reactions can be cleaner and more rapid and economic analyses suggest that the cost of curing polymers may be reduced by switching over to the use of microwaves. This book provides comprehensive coverage of microwave-assisted

polymerization. The first chapter introduces readers to the theory behind the accelerating effects of microwaves on chemical reactions and covers the types of commercial microwave reactors being used for synthesis and processing of polymers that are available on the market. Subsequent chapters are organised by type of reaction, including radical homo and co-polymerizations, step growth polymerization and peptide synthesis. Importantly, analysis of processes and product properties in comparison with conventional methods is also detailed. This book will be a valuable resource for green chemists and polymer scientists and engineers who want to develop sustainable processes.

Historically pharmaceutical and fine chemical products have been synthesised using batch methods, but increasingly chemists are looking towards flow chemistry as a greener and more efficient alternative. In flow chemistry reactions are performed in a reactor with the reactants pumped through it. It has the benefit of being easily scaled up and it is straightforward to integrate synthesis, workup and analysis into one system. Flow chemistry is considered a greener alternative to batch chemistry because it is easier to control and minimise hazardous intermediates and by-products. There is significant interest in the use of flow chemistry both in the lab and on an industrial scale. Flow Chemistry provides an update on recent advances that have been made in the field. Particular emphasis is given to the new integrated approaches that bring together several elements to implement flow processes as a regular green chemistry tool for the chemical industries. With chapter contributions from several well-known experts in the field, this book is a valuable resource for researchers working in green chemistry and synthesis, chemical engineers and industrial chemists working in the pharmaceutical and fine chemicals industries. om several well-known experts in the field, this book is a valuable resource for researchers working in green chemistry and synthesis, chemical engineers and industrial chemists working in the pharmaceutical and fine chemicals industries.om several well-known experts in the field, this book is a valuable resource for researchers working in green chemistry and synthesis, chemical engineers and industrial chemists working in the pharmaceutical and fine chemicals industries.om several well-known experts in the field, this book is a valuable resource for researchers working in green chemistry and synthesis, chemical engineers and industrial chemists working in the pharmaceutical and fine chemicals industries.

Solvents, Surfactants, Solutes and Solids

Presents state-of-the-art knowledge of heterogeneous catalysts including new applications in energy and environmental fields This book focuses on emerging techniques in heterogeneous catalysis, from new methodology for catalysts design and synthesis, surface studies and operando spectroscopies, ab initio techniques, to critical catalytic systems as relevant to energy and the environment. It provides the vision of addressing the foreseeable knowledge gap unfilled by classical knowledge in the field. Heterogeneous Catalysts: Advanced Design, Characterization and Applications begins with an overview on the evolution in catalysts synthesis and introduces readers to facets engineering on catalysts; electrochemical synthesis of nanostructured catalytic thin films; and bandgap engineering of semiconductor photocatalysts. Next, it examines how we are gaining a more precise understanding of catalytic events and materials under working conditions. It covers bridging pressure gap in surface catalytic studies; tomography in catalysts design; and resolving catalyst performance at nanoscale via fluorescence microscopy. Quantum approaches to predicting molecular reactions on catalytic surfaces follows that, along with chapters on Density Functional Theory in heterogeneous catalysis; first principles simulation of electrified interfaces in electrochemistry; and high-throughput computational design of novel catalytic materials. The book also discusses embracing the energy and environmental challenges of the 21st century through heterogeneous catalysis and much more. Presents recent developments in heterogeneous catalysis with emphasis on new fundamentals and emerging techniques Offers a comprehensive look at the important aspects of heterogeneous catalysis Provides an applications-oriented, bottoms-up approach to a high-interest subject that plays a vital role in industry and is widely applied in areas related to energy and environment Heterogeneous Catalysts: Advanced Design, Characterization and Applications is an important book for catalytic chemists, materials scientists, surface chemists, physical chemists, inorganic chemists, chemical engineers, and other professionals working in the chemical industry.

This book presents the latest research in the field of heterogeneous catalysis. Heterogeneous catalysis and homogeneous catalysis are important factors in increasing the development of green chemistry. Some of the challenges that we are responsible for are directing research efforts toward increasing the kinetics of heterogeneous catalysis to homogeneous catalysis levels, improving the recyclability of the catalysts, and developing new supports that can act as catalysts or cocatalysts. Following reaction kinetics and mechanisms on supported catalysts provides the degree of precision and accuracy already enjoyed by the homogeneous catalysis community. The editors present an easily-accessible digest for researchers and a reference aimed at offering guidance to new researchers in the field.

In recent years, a significant amount of progress has been made using green chemistry in the synthesis of synthetically useful compounds and molecules by replacing hazardous chemicals with greener alternatives. However, there is still room for improvement, especially in the pharmaceutical sector where new drugs are being formulated. This book examines green approaches to overcoming hazardous organic transformations. Summarizing recent developments, the book features a detailed description of some of the high impact active pharmaceutical ingredients that have been developed considering green chemistry approaches. It explores the design, engineering and process development and the calculations to account for waste. The book includes strategies to further advance green approaches in the development of generic pharmaceutical industries and features novel, innovative approaches that promote waste-free organic synthesis. This book is of interest to industrialists working in pharmaceuticals and researchers working in green chemistry.

Bringing together a broad range of topics on resource recovery this book provides a valuable resource for those working in green chemistry and waste management.

Globally we are being confronted by the depletion of many natural resources as a result of unsustainable use and increasing global population. Although the debate on the bioeconomy has gained momentum in recent decades, the interest in certifications and standards for biobased products is still weak. This book aims to fill this gap by promoting a holistic approach, which covers environmental, social and economic sustainability aspects and pushes forward the development of a circular, biobased economy. This book promotes the development of sustainability schemes (including standards, labels and certifications) for the assessment of biobased products, which are fundamental to the establishment of a cutting-edge sustainable bioeconomy. Chemical-related, globally relevant case studies are used throughout the book. The content covers a range of issues from upstream and downstream environmental, techno-economic and social assessment, to crosscutting issues such as indirect land use change (iLUC) and end-of-life options. The chapters included in this book will provide a comprehensive review of recent works on life cycle assessment (LCA), life cycle costing (LCC) and social life cycle assessment (s-LCA) methodologies. An important resource for researchers, industrial professionals and policy makers involved in the bioeconomy.

Exploring the range and utility of high-pressure solvent systems across a variety of different chemical applications, this book brings together recent advances in supercritical technology and other pressurised-solvent systems. It provides an in-depth overview of the latest advances and developments and discusses the limitations and drawbacks that need to be addressed. Wherever possible, the greenness and economic viability of the different solvent systems is highlighted. This book is ideal for researchers and industrialists working in environmental science, green chemistry and biorefineries.

In biotechnology and bioengineering, small molecules can be used to increase the efficiency reduce the cost and damage to the environment of certain bioprocesses. This book introduces readers to the important field of chemically promoted biotechnology and bioengineering and presents the theory behind the biotechnology of enzymatic reactions and how they can be chemically enhanced. The book covers chemical modulators for enzymatic reactions, chemically promoted biotechnology in plant cell cultures, chemically promoted biotechnology for plant protection and future prospects for the field. Knowledge gained allows both chemists to make use of biotechnology to solve chemical problems in an environmentally-friendly way, and biologists to make use of chemistry to increase biotechnological efficiency. This book is useful for scientists in a broad range of disciplines, including agricultural chemistry, pesticide science, medicinal chemistry, biochemistry, bio-organic chemistry, cell and molecular biology. Students and researchers in both academia and industry will find it a useful handbook.

Heterogeneous Catalysis for Today's ChallengesSynthesis, Characterization and ApplicationsRoyal Society of Chemistry

Solvents are ubiquitous throughout the chemical industry and are found in many consumer products. As a result, interest in solvents and their environmental impact has been steadily increasing. However, in order to achieve maximum integration of new green solvents into the relevant chemical sectors, clarification of the social, economic, and environmental implications of solvent substitution are needed. This book explores the solvent life cycle, highlighting the challenges faced at various points, from production, through the supply-chain and downstream use to end-of-life treatment. It also discusses the potential benefits that a green chemistry and bio-based economy approach could bring. The current state-of-the-art of green solvents is evaluated along these lines, in addition to reviewing their applications with an appreciation of sustainability criteria. Providing a critical assessment on emerging solvents and featuring case studies and perspectives from different sectors, this is an important reference for academics and industrialists working with solvents, as well as policy-makers involved in bio-based initiatives.

Traditional thermal and freezing processing techniques have been effective in maintaining a safe high quality food supply. However, increasing energy costs and the desire to purchase environmentally responsible products have been a stimulus for the development of alternative technologies. Furthermore, some products can undergo quality loss at high temperatures or freezing, which can be avoided by many alternative processing methods. This second edition of Alternatives to Conventional Food Processing provides a review of the current major technologies that reduce energy cost and reduce environmental impact while maintaining food safety and quality. New technologies have been added and relevant legal issues have been updated. Each major technology available to the food industry is discussed by leading international experts who outline the main principles and applications of each. The degree to which they are already in commercial use and developments needed to extend their use further are addressed. This updated reference will be of interest to academic and industrial scientists and engineers across disciplines in the global food industry and in research, and to those needing information in greener or more sustainable technologies.

An integrated approach to the molecular theory of reaction mechanism in heterogeneous catalysis, largely based on the knowledge among the growing theoretical catalysis community over the past half century, and covering all major catalytic systems. The authors develop a general conceptual framework, including in-depth comparisons with enzyme catalysis, biomineralisation, organometallic and coordination chemistry. A chapter dedicated to molecular electrocatalysis addresses the molecular description of reactions at the liquid-solid interphase, while studies range from a quantum-chemical treatment of individual molecular states to dynamic Monte-Carlo simulations, including the full flexibility of the many-particle systems. Complexity in catalysis is explained in chapters on self-organization and self-assembly of catalysts, and other sections are devoted to evolutionary, combinatorial techniques as well as artificial chemistry.

This book explores the most effective or promising catalytic processes for the conversion of biobased components into high added value products, as platform chemicals and intermediates.

Discussing the broad impact of alternative energy transfer technologies on reactions, separations and materials synthesis, for industrialists, academics and postgraduates in alternative-energy based processing.

This book presents the latest research in the field of heterogeneous catalysis. Heterogeneous catalysis and homogeneous catalysis are important factors in increasing the development of green chemistry. Some of the challenges that we are responsible for are directing research efforts toward increasing the kinetics of heterogeneous catalysis to homogeneous catalysis levels, improving the recyclability of the catalysts, and developing new supports that can act as catalysts or cocatalysts. Following reaction kinetics and mechanisms on supported catalysts provides the degree of precision and accuracy already enjoyed by the homogeneous catalysis community. The editors present an easily-accessible digest for researchers and a reference aimed at offering guidance to new researchers in the field. Priced at £110.00 or US$180.00.

In recent years bioprocessing has increased in popularity and importance, however, bioprocessing still poses various important techno-economic and environmental challenges, such as product yields, excessive energy consumption for separations in highly watery systems, batch operation or the downstream processing bottlenecks in the production of biopharmaceutical products. Many of those challenges can be addressed by application of different process intensification technologies discussed in the present book. The first book dedicated entirely to this area, Intensification of Biobased Processes provides a comprehensive overview of modern process intensification technologies used in bioprocessing. The book focusses on four different categories of biobased products: bio-fuels and platform chemicals; cosmeceuticals; food products; and polymers and advanced materials. It will cover various intensification aspects of the processes concerned, including (bio)reactor intensification; intensification of separation, recovery and formulation operations; and process integration. This is an invaluable source of information for researchers and industrialists working in chemical engineering, biotechnology and process engineering.

It is well-established that organic synthetic processes have been at the core of the chemical industry for hundreds of years, in the production of organic compounds with a wide range of applications. However, we are becoming increasingly aware of the hazardous substances used and generated by these chemical processes. The field of organic synthesis has undergone profound changes to switch to equally efficient, but more sustainable processes that avoid the extensive use of toxic and hazardous reagents and solvents, harsh reaction conditions and expensive and sophisticated catalysts. Explaining methods for carrying out chemical syntheses without the use of catalysts, this book shows how avoiding catalysts during synthesis can mean less use of toxic chemicals, environmentally damaging chemicals or endangered elements and lower costs. It is an important reference for chemists involved in organic synthesis, as well as for green chemists.

In recent years carbon dioxide has played an increasingly important role in biomass processing. This book presents the state-of-the-art of a range of diverse approaches for the use of carbon dioxide in biomass valorisation. The book explores cutting-edge research and important advances in green high-pressure technologies. It gives an overview of the most relevant and promising applications of high-

pressure CO2-based technologies in biomass processing from the perspective of the biorefinery concept. Demonstrating the interdisciplinary aspects of high-pressure technologies from biology, chemistry and biochemical engineering areas, this book brings researchers and industrialists up to date with the latest advances in this field, including novel technologies for energy; biochemicals and materials production; and green chemical engineering processes.

The transportation industry is still largely reliant on fossil fuels, whose use and extraction have significant environmental costs. Biofuels produced from renewable resources biomass offer a more sustainable alternative. However, it is important that production methods should be energy efficient and that feedstocks should not compete with food sources. Biofuels that meet these criteria are sometimes referred to as second-generation biofuels. The new edition of this book provides updates on the three previously discussed non-conventional pathways for second-generation biofuels, including new experimental results and pilot plant studies. It also includes a completely new chapter looking at developments in combining renewable electricity with fuel production and possible future directions for the transportation industry. It is a useful read for researchers and industrialists working in biofuel development as well as postgraduate students studying fuel alternatives.

Rubber is used in a vast number of products, from tyres on vehicles to disposable surgical gloves. Increasingly both manufacturers and legislators are realising that recycling is essential for environmental sustainability and can improve the cost of manufacture. The volume of rubber waste produced globally makes it difficult to manage as accumulated waste rubber, especially in the form of tyres, can pose a significant fire risk. Recycling rubber not only prevents this problem but can produce new materials with desirable properties that virgin rubbers lack. This book presents an up-to-date overview of the fundamental and applied aspects of renewability and recyclability of rubber materials, emphasising existing recycling technologies with significant potential for future applications along with a detailed outline of new technology based processing of rubber to reuse and recycle. This book will be of interest to researchers in both academia and industry as well as postgraduate students working in polymer chemistry, materials processing, materials science and engineering.

The principles of Green Chemistry aim to improve the sustainability of chemical processes and reduce the generation of hazardous substances. There has been great growth in the field over the past few years and the number of research groups working in this area is still increasing. Now one of the biggest challenges is to embed the Green Chemistry ideals of safety and sustainability as standard, both in industry and academia. In order to do this, it is important to create resources that detail different applications and approaches. Green Synthetic Processes and Procedures brings together expert contributors from across a number of areas of green synthesis to cover a diverse array of subjects. Providing a thorough overview of the current green synthetic toolbox, from biocatalysis to sonochemistry, this book is a useful resource for any chemist wishing to design cleaner and safer processes.

The implementation of ionic liquids technologies in future biorefineries is challenging. Different approaches can be applied along the entire chain of biomass valorisation to achieve a specific target molecule, from biomass pre-treatment and fractionation processes to extraction, downstream separation and purification methodologies of high value added products and pivot chemicals. This book summarises recent achievements in the use of ionic liquids in biomass processing as an alternative to conventional processes, particularly in the context of green chemistry. It features real-world case studies where high value-added products have been obtained using ionic liquid processing, demonstrating the practical applications of these technologies. The book concludes by assessing the development of further biorefineries with ionic liquids. The book is an important reference for researchers and practising chemists, bringing readers up-to-date with current research in this field.

Covering topics including solvent selection, miniaturization and metrics for the evaluation of greenness this is a useful resource for researchers interested in reducing the risks and environmental impacts of analytical methods.

New and Future Developments in Catalysis is a package of seven books that compile the latest ideas concerning alternate and renewable energy sources and the role that catalysis plays in converting new renewable feedstock into biofuels and biochemicals. Both homogeneous and heterogeneous catalysts and catalytic processes will be discussed in a unified and comprehensive approach. There will be extensive cross-referencing within all volumes. The use of catalysts in the nanoscale offers various advantages (increased efficiency and less byproducts), and these are discussed in this volume along with the various catalytic processes using nanoparticles. However, this is not without any risks and the safety aspects and effects on humans and the environment are still unknown. The present data as well as future needs are all part of this volume along with the economics involved. Offers in-depth coverage of all catalytic topics of current interest and outlines future challenges and research areas A clear and visual description of all parameters and conditions, enabling the reader to draw conclusions for a particular case Outlines the catalytic processes applicable to energy generation and design of green processes

Fast pyrolysis and related catalytic pyrolysis are of increasing interest as pathways to advanced biofuels that closely mimic traditional petroleum products. Research has moved from empirical investigations to more fundamental studies of pyrolysis mechanisms. Theories on the chemical and physical pathways from plant polymers to pyrolysis products have proliferated as a result. This book brings together the latest developments in pyrolysis science and technology. It examines, reviews and challenges the unresolved and sometimes controversial questions about pyrolysis, helping advance the understanding of this important technology and stimulating discussion on the various competing theories of thermal deconstruction of plant polymers. Beginning with an introduction to the biomass-to-biofuels process via fast pyrolysis and catalytic pyrolysis, chapters address prominent questions such as whether free radicals or concerted reactions dominate deconstruction reactions. Finally, the book concludes with an economic analysis of fast pyrolysis versus catalytic pyrolysis. This book will be of interest to advanced students and researchers interested in the science behind renewable fuel technology, and

particularly the thermochemical processing of biomass.