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Books to drive discovery

From the Royal Society of Chemistry

The print and eBooks in our portfolio number in the hundreds, and all are full of relevant, expert insight from international authors and editors. The information required to take a vital next step – whether in study, research or teaching technique – could come from any one of them. So for 2021, we wanted to highlight recently published titles, as well as giving you advanced notice of the books coming in the next six months.

Refine your ideas

Specialist Periodical Reports can always be relied upon to provide an expertly reviewed, balanced perspective on specific fields in the chemical sciences. The 50th volume in the trusted Organophosphorus Chemistry collection will be published in 2021. An amazing achievement! You can also look forward to the 50th book in our professional reference series Issues in Environmental Science and Technology. *Environmental Pollutant Exposures and Public Health* will join many other popular titles.

Take on global challenges

The world saw rapid change in 2020, and the role of the chemical sciences in combating health challenges faced around the world has been made all the clearer. *The COVID-19 Pandemic and the Future: Virology, Epidemiology, Translational Toxicology and Therapeutics* chronicles the outbreak and worldwide spread of SARS-Cov-2 (COVID-19) and describes the role that several disciplines have to play in therapeutic and control measures.

Try something new

For those of you exploring fresh lines of enquiry, the first books in our Chemistry in the Environment and Drug Development and Pharmaceutical Science series' are on the way in 2021.

And created in partnership with the students who will use them, the Chemistry Student Guides series focuses on and tackles the most challenging aspects of key topics in the chemical sciences.

If you have any queries, contact books@rsc.org to talk to the team.

For a list of books published prior to 2020, visit [rsc.li/backlist](https://www.rsc.li/backlist)

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Catalysis Series

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ISSN 1757-6725

Editor-in-chief

Justin S J Hargreaves University of Glasgow, UK

Series editors

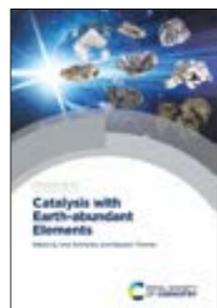
Jose Rodriguez Brookhaven National Laboratory, USA

Catalysis is a major area of scientific research covering numerous fields of chemistry, and is a key factor in tackling many of the scientific challenges faced today, such as renewable energy systems and environmental protection. The books in this series provide an accessible reference for postgraduates, academics and industrialists working in this exciting field. The books cover both the research developments and applications of catalysis, across academia and industry.

Catalysis with Earth-abundant Elements

Uwe Schneider University of Edinburgh, UK | **Stephen Thomas** University of Edinburgh, UK

Catalysis remains a key technology in the 21st century. Considering the limited resources of our planet, earth-abundant elements will have to be explored increasingly in the future. The aim of this book is to highlight the use of the most earth-abundant elements in various types of catalysis and will be of interest to graduates, academic researchers and practitioners in catalysis.



Hardback | 350 pages
9781788011181 | 2021
£169.00 | \$235.00



ISBN 978-1-78801-118-1

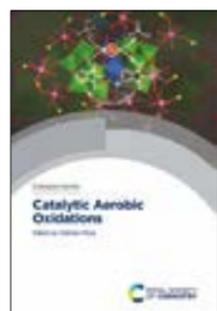


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Catalytic Aerobic Oxidations

Esteban Mejía Leibniz Institute for Catalysis (LIKAT), Germany

Catalytic reactions that are selective and efficient and allow the replacement of common stoichiometric oxidants with molecular oxygen from air at atmospheric pressure provide higher atom efficiency and water as the only side product. Focusing on the use of molecular oxygen as the terminal oxidant, this book covers recent advances in both heterogeneous and homogeneous catalytic systems in academia and industry.



Hardback | 334 pages |
9781788017206 | 2020
£169.00 | \$235.00



ISBN 978-1-78801-720-6



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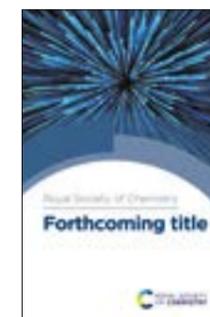
Catalysis Series

Computational Catalysis

2nd Edition

Arvind Asthagiri Ohio State University, USA | **Michael Janik** Pennsylvania State University, USA

Documenting the many advances made possible by improved computing power and new developments in approaches such as machine learning this new edition of Computational Catalysis provides an introduction to, and description of, the up-to-date techniques for first-principles-based modelling of catalysts. Written to be accessible to anyone with a familiarity with quantum mechanical methods, this is a valuable resource for researchers working in both the fields of computational chemistry and catalysis.



Hardback | 300 pages
9781788018814 | 2021
£159.00 | \$220.00



ISBN 978-1-78801-881-4

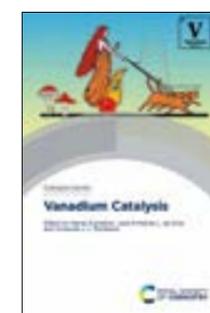


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Vanadium Catalysis

Manas Sutradhar University of Lisbon, Portugal | **Armando J L Pombeiro** University of Lisbon, Portugal | **José Armando L da Silva** University of Lisbon, Portugal

Vanadium is one of the more abundant elements in the Earth's crust making it a more sustainable and more economical choice as a catalyst than many of the noble metals. A wide variety of reactions have been found to be catalysed by both homogeneous and supported vanadium complexes. This book brings together the research on the catalytic uses of this element into one essential resource. Including theoretical perspectives on proposed mechanisms for vanadium catalysis and an overview of its relevance in biological processes.



Hardback | 450 pages
9781788018579 | 2021
£199.00 | \$275.00



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Theoretical and Computational Chemistry Series

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ISSN 2041-3181

Editor-in-chief

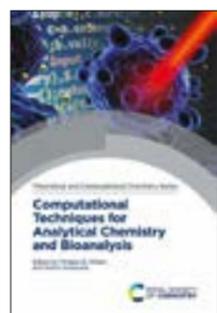
Jonathan Hirst University of Nottingham, UK

Covering all aspects of theoretical and computational chemistry, from current theoretical methods and techniques to new developments in emerging areas, this series comprises up-to-date and timely references for postgraduate students and practising chemists. Books in the series cover both the methodologies at the core of the discipline and applications at the interface with physics, materials, computer science, biological and life sciences. They provide timely, in-depth treatments at the frontiers of theoretical and computational chemistry.

Computational Techniques for Analytical Chemistry and Bioanalysis

Philippe B Wilson Nottingham Trent University, UK | **Martin Grootveld** De Montfort University, UK

As analysis in chemical and biological fields has developed so computational techniques have advanced enabling greater understanding of the data. This work will serve as a definitive overview of the field of computational simulation as applied to analytical chemistry and biology, drawing on recent advances as well as describing essential, established theory. Computational approaches provide additional depth to biochemical problems, as well as offering alternative explanations to atomic scale phenomena. Highlighting the innovative and wide-ranging breakthroughs made by leaders in computational spectrum prediction and the application of computational methodologies to analytical science, this book is for graduates and postgraduate researchers showing how computational analytical methods have become accessible across disciplines.



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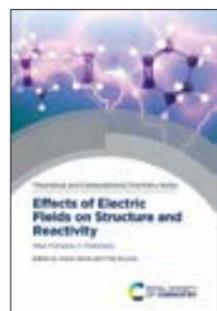
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Effects of Electric Fields on Structure and Reactivity

New Horizons in Chemistry

Sason Shaik The Hebrew University of Jerusalem, Israel | **Thijs Stuyver** The Hebrew University of Jerusalem, Israel

Written by leaders in the field, Effects of Electric Fields on structure and Reactivity is the first book on this exciting topic. Starting with an overview of the theory behind the effect of electric fields on chemical structure and reactivity, this accessible reference work aims to encourage those new to the field to consider harnessing these effects in their own work. Covering applications and recent theoretical developments, it is a useful resource for theoretical chemists and experimentalists alike.



Hardback | 490 pages
9781839161698 | 2021
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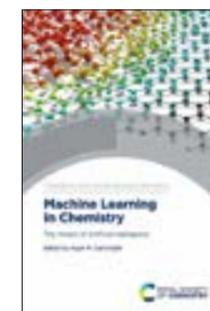
Theoretical and Computational Chemistry Series

Machine Learning in Chemistry

The Impact of Artificial Intelligence

Hugh M Cartwright Oxford University (retired), UK

There is a growing consensus that machine learning (ML) has the potential to develop into a tool that is almost as fundamental in scientific research as computers themselves. With contributions from leading research groups, this book presents in-depth examples of the application of ML to real chemical problems. Through these examples, readers who are intrigued by the power of this technique can gain a feel for its potential and discover how it might be applied in their own field.



Hardback | 546 pages
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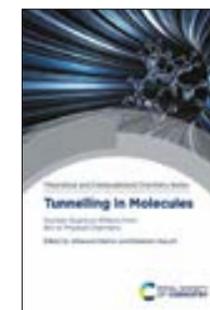
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Tunnelling in Molecules

Nuclear Quantum Effects from Bio to Physical Chemistry

Johannes Kästner University of Stuttgart, Germany | **Sebastian Kozuch** Ben-Gurion University of the Negev, Israel

The field of quantum tunnelling has been rapidly developing in the 21st century, yet there are no updated books on its applications in chemistry. Including theoretical and experimental chapters, from the physical and organic to the biochemistry fields, this new book provides a broad and conceptual perspective of the reactivity of molecules lead by quantum mechanical tunnelling.



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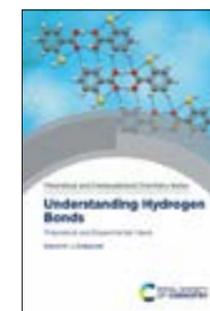
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Understanding Hydrogen Bonds

Theoretical and Experimental Views

Stawomir J Grabowski University of the Basque Country and Donostia International Physics Center (DIPC), Spain

The area of hydrogen bonding is one that is well studied, but our understanding continues to develop as the power of both computational and experimental techniques has improved. This book presents an up-to-date overview of our theoretical and experimental understanding of the hydrogen bond. It covers both well-established and novel approaches, new types of interaction that might be classified as hydrogen bonds and a comparison of hydrogen bonds to other types of non-covalent interactions.



Hardback | 450 pages
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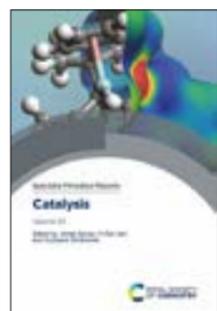
Specialist Periodical Reports

Catalysis

Volume 33

James Spivey Louisiana State University, USA | **Yi-Fan Han** East China University of Science and Technology, China | **Dushyant Shekhawat** National Energy Technology Laboratory, USA

This volume looks at modern approaches to catalysis and reviews the extensive literature. Chapters highlight application of 2D materials in biomass conversion catalysis, plasmonic photocatalysis, catalytic demonstration of mesoporosity in the hierarchical zeolite and the effect of surface phase oxides on supported metals and catalysis. Looking to the future a chapter on ab initio machine learning for accelerating catalytic materials discovery is included. Appealing broadly to researchers in academia and industry, these illustrative chapters bridge the gap from academic studies in the laboratory to practical applications in industry not only for catalysis field but also for environmental protection. The book will be of great benefit to any researcher wanting a succinct reference on developments in this area now and looking to the future.



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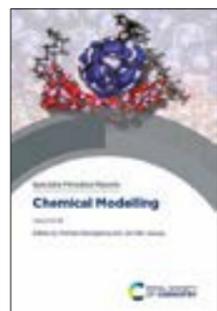
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Chemical Modelling

Volume 16

Michael Springborg University of Saarland, Germany | **Jan-Ole Joswig** Dresden University of Technology, Germany

Chemical modelling covers a wide range of disciplines and this book is the first stop for any materials scientist, biochemist, chemist or molecular physicist wishing to acquaint themselves with major developments in the applications and theory of chemical modelling. Containing both comprehensive and critical reviews, this volume is a convenient reference to the current literature.



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Professional Reference

Determining Stability Constants

A Handbook

Pall Thordarson University of New South Wales, Australia

Determining binding constants is a fundamental component of experimental chemistry research. This book provides an up-to-date overview of the most powerful experimental methods and software tools available and systematically catalogues the main methods and useful information regarding the determination of stability constants in supramolecular chemistry, ranging from simple host-guest equilibria to complex cooperative assemblies. Written by an expert in the field, this title will be an important resource for students and researchers working in supramolecular chemistry, inorganic chemistry and drug delivery.



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Faraday Discussions

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ISSN 1359-6640

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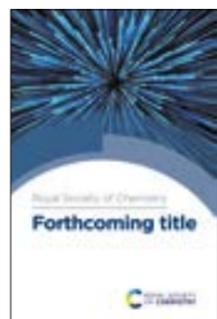
David Lennon University of Glasgow, UK | **Angelos Michaelides** University College London, UK | **Jenny Nelson** Imperial College London, UK | **Susan Perkin** University of Oxford, UK | **Claire Vallance** University of Oxford, UK

Faraday Discussions covers a variety of topics in rapidly developing areas of the physical sciences, with a focus on physical chemistry and its interfaces with other scientific disciplines. The journal publishes the papers presented and a record of the questions, discussion and debate that took place at the corresponding Faraday Discussions meeting and provides an important record of current international knowledge and opinions in the relevant field. Each Faraday Discussion covers a topic in a rapidly developing area of chemistry, and will be of interest to academic and industrial chemists across all areas of the chemical sciences.

Air Quality in Megacities

Faraday Discussion

Very high levels of pollution are regularly observed in cities across the world. Predicting urban air quality demands detailed knowledge of both the physical properties of the urban atmosphere and pollutants within it, and the chemical reactions, which can transform one pollutant into another. This Faraday Discussion looks at the underlying processes responsible; an essential pre-requisite to developing the high quality numerical models of urban air pollutants, which are required to develop and test mitigation strategies prior to implementation.



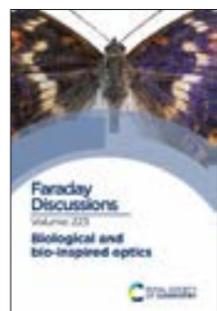
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Over the last decade, an increasingly advanced understanding of nature's light manipulation strategies has allowed scientists and engineers to design novel biologically inspired photonic materials for a wide range of applications. This Faraday Discussion focusses on the most recent developments in this exciting and rapidly evolving field, assessing our current knowledge of natural light management techniques, discussing the application of this knowledge for bio-inspired materials and looking to the future of the field.



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Graphene has extraordinary chemical and physical properties ensuring its use in opto-electronics, energy and biomedical applications. One of the greatest challenges is to develop and master chemical strategies for other 2D materials such as transition metal dichalcogenides. This Faraday Discussion covers all areas related to other 2D materials' chemistry spanning from their theoretical/computational prediction to their synthesis and functionalization yielding 2D and 3D systems with tailor made physical properties for a wide range of applications.



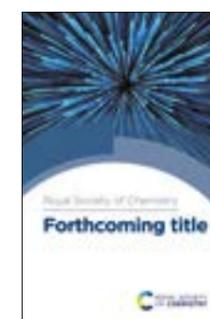
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There has been exponential growth in the number of nanoporous framework materials reported in the scientific literature over recent years. These novel families of materials open up new horizons in practically all branches of engineering, physics, chemistry, biology, and medicine. With their numerous applications as selective adsorbents and catalysts, substrates for biosensors and drug delivery, membranes and films in various nanotechnologies this Faraday Discussion discusses both the fundamentals and the applied aspects of framework materials.



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Luminescent Silicon Nanostructures

Faraday Discussion 222

Silicon is the most important semiconducting material of the microelectronic industry. Bulk silicon does not exhibit good optical properties, however in the late 1980s good emission was observed in porous silicon. Since then, a variety of luminescent silicon nanostructures have been investigated, but the origin of this luminescence is debated in the literature. This Faraday Discussion explores new methodologies to synthesize and characterise luminescent silicon nanostructures, from porous silicon to nanocrystals and nanorods.



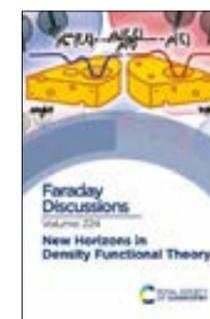
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Density functional theory (DFT) is today's most widely used method for practical computational electronic structure calculations across chemistry, physics and materials science. Fuelled by a rapid increase in computational power and the advent of linear scaling technologies the systems to which DFT may be applied have become ever larger, more complex. This Faraday Discussion brings together chemists, physicists, materials scientists and applied mathematicians who develop new density-functional methods and rely on this approach as a key tool in their research.



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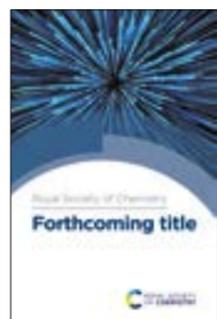


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Reaction Mechanisms in Catalysis

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Heterogeneous catalysis is a core area of contemporary physical chemistry posing major fundamental and conceptual challenges. It lies at the heart of the chemical industry - an immensely successful and important part of the overall UK economy, and catalysis plays a crucial part in the production of 80% of all manufactured goods. This Faraday Discussion discusses key aspects of reaction mechanism studies and how this can drive rational design of catalysts.



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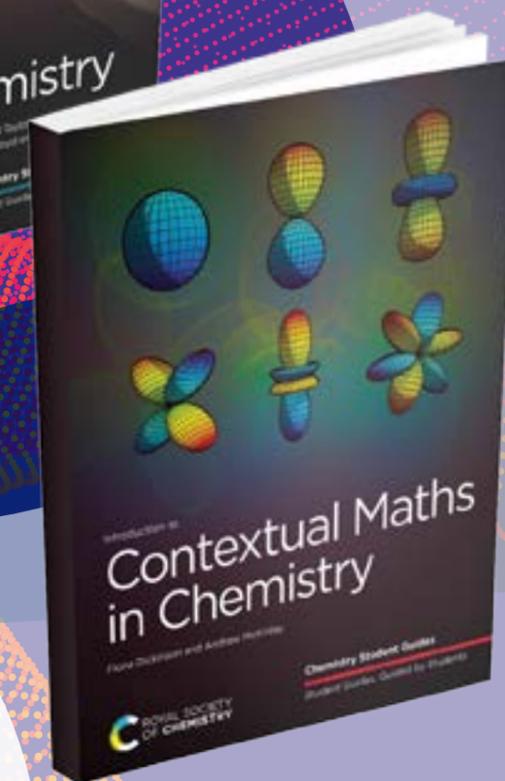
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