



# Physical chemistry

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Written by internationally recognised authors, our physical chemistry books provide in-depth, reliable information on the ever-expanding range of subjects at the interface of physical chemistry and, chemical physics. In 2019 look out for the latest research in catalysis, and computational techniques.

## Five minutes with...



**Name** Cerys Willoughby

**Affiliation** University of Southampton, UK

**Author of** *Recording Science in the Digital Era*

**Book publication date** September 2019

**ISBN** 9781788014205

### Tell us about your book

For most of the history of scientific endeavour, science has been recorded on paper. In this digital era, however, there is increasing pressure to abandon paper in favour of digital tools. This book examines the importance of record-keeping in science, current record-keeping practices, and the role of technology for enabling the effective capture, storage, sharing, and preservation of scientific data. It focuses on the roles and design of Electronic Laboratory Notebooks (ELNs) and data management systems in particular, including an in-depth discussion of the barriers and potential pitfalls of these technologies together with some best practices for overcoming them.

### What do you think will be the next big breakthrough in your subject area?

Personally, I think being able to use digital tools in a more naturalistic way will help to encourage adoption. Writing and drawing in a notebook is very easy and natural, but recording on a computer is harder. Now we are beginning to get interfaces, that allow detailed writing and drawing. Future developments could enable the user to talk directly to the ELN to call up previous results or to dictate observations and measurements during an experiment. Another area where I think important developments will be made is in the interaction between ELNs and other systems. I think there is huge value to be gained by enabling users to click a button that automatically packages and uploads all the appropriate data, metadata, and documentation for a research project directly to a repository or publisher.

### What is the current take up of ELN and how has it been received?

The take up of ELNs is variable across different sectors. Although ELNs are widely used in industry, they are by no means ubiquitous. Within academia there is a lot of interest in implementing ELNs, but most researchers are still recording their research using paper notebooks. There are a number of challenges with ELNs, common concerns are the cost of licenses, issues around where the data is stored for privacy and security reasons, and the usability of the software itself. In my experience, users who collaborate in their research are most positive, but other users only become positive once they use them and see the benefits of being able to easily organise and access their research.

### Looking back what is the biggest development in your area of research?

There has been gradual progress over a long period of time, but I think the most significant is probably the development of web-based ELNs, particularly those using the Cloud. Although these are not suitable for all organisations, they are useful for individuals, small teams, and those wanting to try out ELNs. Many of the online ELNs are free to use or have a free trial option. The majority are quite generic, and can potentially be used by any discipline, overcoming the inflexibility of some of the more complex ELNs available. The generic design also means they tend to be relatively easy to use. Having the content accessible from anywhere, including on mobile, also provides the flexibility to create content without being tied to a particular machine that has an appropriate license.

## Five minutes with...



**Name** Kamran T Mahmudov

**Affiliation** University of Lisbon, Portugal

**Co-editor of** *Noncovalent Interactions in Catalysis*

**Book publication date** April 2019

**ISBN** 9781788014687

### Tell us about your book

Noncovalent interactions can have an important impact on the energetics and structures of molecules, as well as on their reactivity and on the selectivity of their reactions. In fact, these weak forces can play an essential role in the action of nature's catalysts, enzymes, (as well as in organocatalysis, metal catalysed systems, cooperative catalysis, etc.), namely by lowering the kinetic barriers of reactions through transition state stabilisation(s). The crucial role of the majority of types of noncovalent interactions in the stabilisation of intermediates is highlighted in both homogenous and heterogeneous catalyses. We believe the book will be useful for synthetic chemists that are interested in the design of catalysts and discovery of new catalytic reaction pathways.

### What do you think will be the next big breakthrough in your subject area?

A catalyst can bring reactants together and promote their reaction by noncovalent interactions (e.g., involving a transition state). Among these weak forces, hydrogen bonding, cation- $\pi$  and anion- $\pi$  interactions have already been well explored in some types of reactions of organocatalysis. We believe that other types of catalytic reactions, namely in cooperative catalysis and transition-metal catalysis, will also be found to be effectively assisted by noncovalent interactions. Additionally, other forms of noncovalent interactions, such as  $\sigma$ -hole bonds, could in the future hold an important position in synthesis and catalysis. We expect that the catalysis of this century will be largely driven by noncovalent interactions.

### What was the biggest challenge you faced when writing your book?

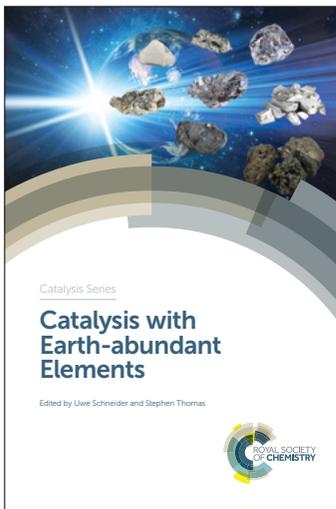
The biggest challenge was to gather internationally renowned scientists, in the various areas of expertise, with complementary viewpoints, to cover all the important and promising fields concerning noncovalent interactions in catalysis. I'd like to take this opportunity to thank all the authors who accepted our invitation for their excellent contributions.



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## About the series

ISSN: 1757-6725

### Editor-in-chief

**Justin S J Hargreaves** University of Glasgow, UK

### Series editors

**Jose Rodriguez** Brookhaven National Laboratory, USA | **Bert Klein Gebbink** Utrecht University, The Netherlands

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 | 2018 | £169.00 | \$235.00



## Enantioselective Cobalt-catalysed Transformations



**Hélène Pellissier** CNRS, France

Cobalt catalysts are a cheaper, more environmentally responsible alternative to many of the more commonly used transition metal catalysts. This book collects the major developments reported in the past thirty years in the field of enantioselective reactions promoted by chiral cobalt catalysts. It is a useful reference resource for chemists, both academic and industrial, working in organic synthesis and interested in greener or more economical catalytic alternatives.

Hardback | 224 pages | 9781788014625 | 2018 | £123.00 | \$170.00





## Nanoparticle Design and Synthesis for Catalytic Applications

Rafael Luque University of Córdoba, Spain | Pepijn Prinsen University of Córdoba, Spain



Nanoparticles exhibit a range of different properties when compared to bulk materials. Their high surface-area to volume ratio makes them particularly attractive for use as catalysts and recent years have seen an explosion of research in this area. This book presents an introduction to the preparation and characterisation of nanomaterials and their design for specific catalytic applications. It is a valuable resource for researchers working on catalytic reactions, industrial processes and nanomaterial applications.

Hardback | 270 pages | 9781788014908 | 2019 | £149.00 | \$205.00

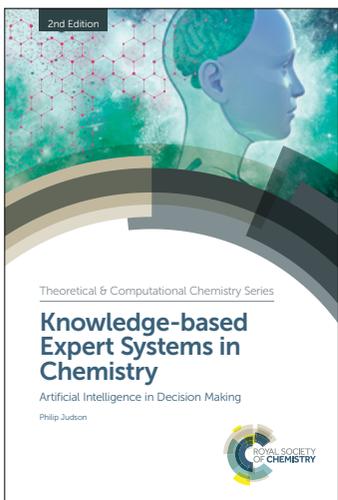
## Noncovalent Interactions in Catalysis

Kamran T Mahmudov University of Lisbon, Portugal | Maximilian N Kopylovich University of Lisbon, Portugal | M Fatima C Guedes da Silva University of Lisbon, Portugal | Armando Pombeiro University of Lisbon, Portugal



Noncovalent interactions (such as hydrogen bonds,  $\pi$ - $\pi$  stacking and lipophilic interactions) often provide the spine of biomolecular and material structures, and can therefore play a key role in biological and catalytic processes. This book provides an overview of the role of different types of noncovalent interactions in both homogenous and heterogeneous catalysis. With chapters contributed by experts from around the world it is a valuable resource for synthetic chemists who are interested in exploring and further developing noncovalent interaction-assisted synthesis and catalysis.

Hardback | 500 pages | 9781788014687 | 2019 | £179.00 | \$250.00



## About the series

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** De Montfort 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.

Hardback | 500 pages | 9781788014618 | 2019 | £179.00 | \$250.00



## Knowledge-based Expert Systems in Chemistry



Artificial Intelligence in Decision Making

2nd Edition

**Philip Judson** Consultant, Harrogate, UK

There have been significant developments in the use of knowledge-based expert systems in chemistry since the first edition of this book was published in 2009. This new edition has been thoroughly revised and updated to reflect the advances. Written by a pioneer in the field, this book provides an essential reference for anyone interested in the uses of artificial intelligence for decision making in chemistry.

Hardback | 250 pages | 9781788014717 | 2019 | £149.00 | \$205.00





# London Dispersion Forces in Molecules, Solids and Nano-Structures



## An Introduction to Physical Models and Computational Methods

**Janos Angyan** University of Lorraine, France | **John Dobson** Griffith University, Australia | **Georg Jansen** University of Duisburg-Essen, Germany | **Tim Gould** Griffith University, Australia

Summarising current understanding of the physical origin and modelling of London dispersion forces manifested at an atomic level, this book provides theoretical, physical and synthetic chemists, as well as solid-state physicists, with a systematic understanding of the origins and consequences of these ubiquitous interactions. It covers a wide range of system, from small intermolecular complexes, to organic molecules and crystalline solids, through to biological macromolecules and nanostructures.

Hardback | 450 pages | 9781782620457 | 2019 | £179.00 | \$250.00

ISBN 978-1-78262-045-7



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### Catalysis

#### Volume 31

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

Catalysts are required for a variety of applications and industrialists and academics are increasingly challenged to find cost effective and environmentally benign catalysts to use. This volume looks at modern approaches to catalysis and reviews the extensive literature including direct methane conversion, nanocomposite catalysts for transformation of biofuels into syngas and hydrogen and catalytic wet air oxidation technology for industrial wastewater treatment.

Hardback | 300 pages | 9781788014540 | 2019 | £314.95 | \$440.00



### Chemical Modelling

#### Volume 15

**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.

Hardback | 300 pages | 9781788013697 | 2019 | £314.95 | \$440.00



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#### Volume 16

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Providing the reader with an up to date digest of the most important research currently carried out in the field, Electrochemistry Volume 16 is compiled and written by leading experts from across the globe. This volume is a key reference for researchers providing a timely overview of this exciting and developing area.

Hardback | 250 pages | 9781788016926 | 2020 | £314.95 | \$440.00



### Photochemistry

#### Volume 47

**Angelo Albini** University of Pavia, Italy | **Stefano Protti** University of Pavia, Italy

Reviewing photo-induced processes that have relevance to a wide-ranging number of academic and commercial disciplines, this volume reflects the current interests in chemistry, physics, biology and technology. Highlight chapters include the molecules of colour, solar photocatalysis, photochemistry in cryogenic matrices, photoresponsive hydrogels and molecular photoswitches. Essential reading for postgraduates, academics and industrialists working in the field of photochemistry, enabling them to keep on top of the literature.

Hardback | 400 pages | 9781788015547 | 2019 | £314.95 | \$440.00



### Determining Stability Constants

#### A Handbook

Palli 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.

Hardback | 400 pages | 9781788011655 | 2020 | £125.00 | \$175.00



### Optimal Experimental Design for Chemical Engineers

#### Mechanistic Model-based Design with Case Studies

Federico Galvanin University College London, UK

Model building procedures have been proposed for developing, improving and validating mechanistic models in more efficient ways by managing and guiding the information obtained from experimental activities. These procedures heavily rely on the use of efficient computational techniques for model identification based on the use of optimal design of experiments techniques. This book guides the reader through statistical tools and methods for building mechanistic mathematical models in chemical engineering using design of experiment techniques. Relevant chemical engineering case studies are used throughout the book to provide a practical approach to this complex topic. Ideal for experimenters, who will find useful tips for driving experiments, and modellers who will find useful information on model development, selection and validation, this book is essential for chemical engineers across academia and industry.

Hardback | 450 pages | 9781788010870 | 2019 | £179.00 | \$250.00

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### Recording Science in the Digital Era

#### From Paper to Electronic Notebooks and Other Digital Tools

Cerys Willoughby University of Southampton, UK

Electronic lab notebooks (ELNs) are tools that allow experimental protocols and data to be captured digitally; they are analogous to the more traditional paper and pen. In theory, they make it easier to capture, store and share experimental data. However, adoption has been slow in the academic sector. This book provides a description of how and why scientists record data, an overview of the current ELN technology available and the benefits and pitfalls of using them for those interested in implementing digital data solutions within their research groups or departments.

Hardback | 280 pages | 9781788014205 | 2019 | £70.00 | \$95.00



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