### Computational Materials Discovery

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Until a few years ago, new materials could only be discovered experimentally. Now the situation is dramatically different with advances in computational techniques. This is the first book to provide a systematic review of computational materials discovery, covering different methods and materials discovery for specific classes of materials including low-dimensional materials. The book is a convenient introduction for young researchers and industrial scientists to the topic of computational materials design.

**Hardback | 456 pages | ISBN 9781782629610 | £169.00 | $235.00 | 02/11/2018**

### Data Integrity and Data Governance

Practical Implementation in Regulated Laboratories

R D McDowall, Director, R.D.McDowall Ltd

Data integrity is the hottest topic in the pharmaceutical industry at the moment. Global regulatory agencies have issued six guidance documents in the past couple of years, however all documents are vague and do not contain detailed examples or advice to help regulated laboratories to implement policies, procedures and processes to ensure integrity. The aim of this book is to provide practical and detailed advice on how to implement data governance and data integrity for regulated analytical laboratories working in the pharmaceutical and allied industries. It is designed for analytical chemists and scientists working in regulated laboratories, management and senior management roles, primarily in the pharmaceutical industry and consultants who will benefit from the practical guidance provided.

**Hardback | 598 pages | ISBN 9781788012812 | £125.00 | $175.00 | 09/11/2018**

### Electron Paramagnetic Resonance

Volume 26

Victor Chechik, University of York, UK  
Damien M Murphy, University of Cardiff, UK

The topics covered in this volume describe contrasting types of Electron Paramagnetic Resonance (EPR) application, which remain very significant in modern science. This volume compiles critical coverage of developments in the recent literature by a hand-picked group of researchers at the cutting edge of the field. Providing a snapshot of the area, this book is a useful addition to any library supporting this research.

**Hardback | 170 pages | ISBN 9781788013727 | £314.95 | $441.00 | 06/11/2018**

All information is subject to change without notice
Organic Catalysis for Polymerisation
Andrew Dove University of Birmingham, UK
Haritz Sardon University of the Basque Country UPV/EHU, Spain
Stefan Naumann University of Stuttgart, Germany

In recent years polymerisation using organocatalysts has become an appealing alternative to more traditional metal-based catalysts. This book provides a complimentary view of the field, with both an overview of state-of-the-art catalyst development as well as the best methodologies available to create specific polymer types. Edited by leading figures in the field, this title will serve as an excellent reference for postgraduate students and researchers in both academia and industry interested in polymer chemistry, organic chemistry, catalysis and materials science.

Hardback | 648 pages | ISBN 9781788011846 | £199.00 | $275.00 | 22/11/2018

Raman Spectroscopy in Archaeology and Art History
Volume 2
Peter Vandenabeele University of Ghent, Belgium
Howell Edwards University of Bradford, UK

Ten years after the first volume, this book highlights the important contribution Raman spectroscopy makes as a non-destructive method for characterising the chemical composition of objects with archaeological and historical importance. The original book was groundbreaking in its concept, but the last ten years has seen some advancement into new areas, consolidation of some of the older ones and novel applications involving portable instrumentation, on-site in museums and in the field. This new volume maintains the topic at the cutting edge with the Editors having approached prominent contributors to provide case studies. Aimed at scientists involved in conservation, conservators/curators who want to better understand their collections at a material level and researchers of cultural heritage.

Hardback | 349 pages | ISBN 9781788011389 | £199.00 | $279.00 | 01/11/2018

Kinase Drug Discovery
Modern Approaches
Richard A Ward AstraZeneca, UK
Frederick W Goldberg AstraZeneca, UK

Kinase targets and drugs remain an area of significant interest across academia and in the pharmaceutical industry. There are now many marketed drugs which target kinases and a growing number of compounds are currently in various stages of clinical development. This book covers the key areas for kinase inhibition that will be important over the coming years. This will be an important reference for scientists involved in drug discovery in academia or industry, particularly in oncology research.

Hardback | 413 pages | ISBN 9781788010832 | £169.00 | $235.00 | 06/11/2018
Organometallic Chemistry
Volume 42
Nathan J Patmore University of Huddersfield, UK
Paul I P Elliott University of Huddersfield, UK

With the increase in volume, velocity and variety of information, researchers can find it difficult to keep up to date with the literature in their field. This interdisciplinary field has the potential to provide answers to problems and challenges faced in catalysis, synthetic organic chemistry and the development of therapeutic agents and new materials. Providing an invaluable volume, this volume contains analysed, evaluated and distilled information on the latest in organometallic chemistry research.

Hardback | 190 pages | ISBN 97817888010054 | £314.95 | $441.00 | 28/11/2018

Plastics and the Environment
R M Harrison University of Birmingham, UK
R E Hester University of York, UK

As the call to ban plastic microbeads from cosmetics grows, Plastics and the Environment casts a timely light over the societal usage and potential environmental impact of plastics. Written by leading experts, this book provides a scientifically informed overview of the key issues surrounding the topic, from discussions on marine litter, to the impact on wildlife and human exposure. Aimed at policy makers, students, environmental scientists and thinkers, it is an important review that will bring the reader right up to date.

Hardback | 192 pages | ISBN 97817888012416 | £70.00 | $98.00 | 23/11/2018

The Science of Chocolate
Stephen T Beckett

Now in its third edition, this bestselling book describes the complete chocolate making process from growing the beans to the sale in the shops. It has been ten years since the last edition was published and Stephen Beckett has improved and expanded the text to bring it up to date. Revisions include a new chapter 'How do they make that?' which details, for example, how air is incorporated into Aero, how chocolate shapes are filled and other distinctive products. This popular title will appeal to anyone with a fascination for chocolate including food scientists and those working in the confectionery industry.

Paperback | 284 pages | ISBN 97817888012355 | £26.99 | $38.00 | 15/11/2018
Methods and Applications of Crystal Structure Prediction
Faraday Discussion 211

The prediction of crystal structures from first principles has been one of the grand challenges for computational methods in chemistry and materials science. They have been used to study organic molecules such as polymorphism of pharmaceutical molecules or inorganic materials where the discovery and computational design are necessary. However, the communities addressing methods and applications in organic and inorganic crystal structure prediction have largely remained separate, due to the different approaches that have been used in these two areas. This book will encompass the cross-fertilisation of ideas and methods that result from a Faraday Discussion meeting which brought together these theoreticians and interested experimentalists. It will appeal to researchers from computational chemistry, crystallography and crystal engineering and materials science in the development of methods.

Hardback | 668 pages | ISBN 9781788011709 | £170.00 | $238.00 | 15/11/2018

Self-organized Motion
Physicochemical Design based on Nonlinear Dynamics
Satoshi Nakata Hiroshima University, Japan
Véronique Pimienta University of Toulouse, France
István Lagzi Budapest University of Technology and Economics, Hungary
Hiroyuki Kitahata Chiba University, Japan
Nobuhiko J Suematsu Meiji University, Japan

The book gives an overview of the self-propelled motion of chemical objects far from their thermodynamic equilibrium at various spatial scales and its applications. The book will discuss theoretical aspects, the characteristics of the motion, and design procedures of such systems from the viewpoint of nonlinear dynamics. The book is suitable for graduate students and researchers interested in physical and theoretical chemistry as well as soft matter.

Hardback | 372 pages | ISBN 9781788011662 | £169.00 | $235.00 | 06/11/2018