Synopsis
With a strong focus on theory, this book is an up-to-date review of photoelectrochemical water splitting. The book discusses prediction of band alignments, the discovery of novel materials with attractive band gaps and stability; recent developments such as protective overlayers for photoanodes and in operando X-ray measurements of PEC cells; and concludes with a systems analysis of photoelectrochemical water splitting technologies. It is an important reference for researchers working in solar fuels as well as those working in theoretical chemistry.

Brief Contents
- The Challenge of Water Splitting in View of Photosynthetic Reality and of Research Trends
- Theoretical Design of PEC Materials
- Computational Screening of Materials for Photoelectrochemical Water Splitting
- Ab Initio Modeling of Solid-Liquid Interfaces
- Unravelling The Charge Transfer Mechanism in Water Splitting
- Hematite Photoanodes
- Rate Law Analysis of Water Splitting Photoelectrodes
- Solution Processed Electrodes for PEC Water Splitting

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Chemical Modelling

Volume 14

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

Synopsis
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.

Brief Contents
- Theoretical studies as a tool for understanding the aromatic character of porphyrinoid compounds
- Atomistic modeling for molecular electronics and spintronics: successes and challenges
- Recent progress on fermionic exchange symmetry
- Dynamics and electronic structure of atomic clusters
- Clusters as Catalysts: Advantages
- Challenges
- Modeling the oxidation mechanism of pyrite and arsenopyrite - connection to acid rock drainage

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Synopsis
Formaldehyde is virtually ubiquitous in the modern environment due to its cost-effective nature, its use in resin formation, and its preservative properties. Though formaldehyde is necessary for many products and processes important to the world’s economy, this economic dependence on formaldehyde comes at a cost to public health. Scientific inquiry into formaldehyde exposure has grown in response to this public health problem. This book consolidates these developments and will be a valuable source of information for postgraduates and researchers in environmental and occupational exposure as well as regulators.

Brief Contents
- Introduction to Formaldehyde
- Formaldehyde Exposure, Regulation, and Metabolism
- Formaldehyde Exposure in China
- General Toxicity of Formaldehyde
- Formaldehyde Carcinogenesis
- Formaldehyde Exposure and Leukemia Risk
- Potential Mechanisms of Formaldehyde-Induced Leukemia
- Formaldehyde Induced Leukemia-Specific Chromosomal Aneuploidy
- Formaldehyde-Associated Brain Tumors
- Formaldehyde-Associated Neurodegenerative Diseases
Modern Biocatalysis
Advances Towards Synthetic Biological Systems

Gavin Williams North Carolina State University, USA
Mélanie Hall University of Graz, Austria

Synopsis
Surveying current state-of-the-art techniques, this book provides a comprehensive overview of this exciting field. The book focuses on modern techniques that generate better performing enzymatic systems and novel biosynthetic routes to (non-)natural products. This includes the use of molecular techniques in protein design and engineering, the construction of artificial metabolic pathways and the application of computational methods for enzyme discovery and design. The book provides researchers with a greater understanding of current and emerging trends in biocatalysis.

Brief Contents
- Genome Mining for Enzyme Discovery
- De Novo Enzymes
- Artificial Metalloenzymes
- Exploiting Natural Diversity for Industrial Enzymatic Applications
- New Biotools for the Development of Novel Biocatalysts
- Exploiting Computational Techniques for Better Understanding of Enzyme Catalysis
- Mechanistic Insights into Enzymatic Conversion of Biomass
- Modulating Enzyme Activity via Incorporation of Non-canonical Amino Acids

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Non-extractable Polyphenols and Carotenoids

Importance in Human Nutrition and Health

Fulgencio Saura-Calixto ICTAN-CSIC, Spain
Jara Pérez-Jiménez ICTAN-CSIC, Spain

Synopsis

Polyphenols and carotenoids are abundant in fruits, vegetables, herbs and spices, and beverages, such as tea, cocoa and wine providing health-related benefits and antioxidant properties. Focusing on non-extractable polyphenols (NEPP) that are present in the diet, this book will improve our knowledge of dietary intakes and physiological properties of NEPP ensuring a better understanding of their potential health effects. With global appeal, this will be the first book dedicated to raising the profile of this important area. Summarising the current knowledge in the field, the book will direct further research for food chemists, scientists and nutritionists looking for a new perspectives.

Brief Contents

The Story of the Introduction of Non-extractable Polyphenols into Polyphenol Research: Origin, Development and Perspectives
Dietary Fiber and Non-Extractable Polyphenols
Extractable and Non-extractable Polyphenols: An overview
Analysis of Non-extractable Polyphenols (NEPP)
Dietary Sources and Intakes of Non-Extractable Polyphenols
Non-Extractable Polyphenols in Tropical Fruits: Occurrence and Health-related Properties
Fruit and Vegetable Processing: Effects on Extractable and Non-extractable Polyphenols