Computational Studies of Transition Metal Nanoalloys

The focus of this thesis is the computational modelling of transition metal bimetallic (nanoalloy) clusters. More specifically, the study of Pd-Pt, Pt-Pt, Au-Au and Pd-Au as a few tens of atoms in the gas phase. The author used a combination of global optimization techniques - coupled with a Gupta-type empirical many-body potential - and Density Functional Theory (DFT) calculations to study the structures, bonding and chemical ordering, as well as to investigate the chemisorptions of hydrogen and carbon monoxide on bimetallic clusters. This research is highly relevant to experimental catalytic studies and has resulted in more than seven publications in international journals.

Features
- Nominated by the University of Birmingham, UK for a Springer Theses Prize
- Results are relevant for theoretical and experimental studies of nanoalloy cluster structure and heterogeneous catalysis by bimetallic nanoparticles
- The research is also applicable in technological applications of nanoalloys, such as in sensors, optics and magnets

Contents

Fields of interest
Theoretical and Computational Chemistry; Nanochemistry; Catalysis

Target groups
Research

Discount group
P

New Frontiers in Chemical Biology

Enabling Drug Discovery

Despite ever increasing research investment, there has been a decline in the number of new drug approvals over the last decade. In order to improve productivity, the drug discovery community is exploring alternative approaches. The emerging field of chemical biology utilizes the tools and techniques of chemical synthesis to study and influence biochemical systems. It has already led to the identification of novel therapeutic targets and will continue to facilitate drug discovery in the 21st century. This book highlights the new frontiers in chemical biology and describes their impact and future potential. It provides a valuable resource for scientists in academia and industry who are looking to build their knowledge of this hot topic.

Features
- Written by experts
- Presents a comprehensive survey of the field
- Highlights latest developments in the field

Contents

Fields of interest
Medicinal Chemistry; Proteomics; Physical Chemistry

Target groups
Research

Discount group
P

Olefin Upgrading Catalysis by Nitrogen-based Metal Complexes II

State of the art and Perspectives

Olefin Upgrading Catalysis by Nitrogen-based Metal Complexes II: State-of-the-art and Perspectives provides a critical review of the state-of-the-art developments in industrially relevant processes connected to efficient and selective olefin upgrading. Specific attention is devoted to catalysts containing imine- and amine-based ligands. All the chapters in this book have been designed to provide a systematic account of the vast amount of information available for this type of catalyst as well as to highlight the factors that ultimately control the catalyst’s performance and productivity.

Features
- Introduces new concepts
- Contributions from international experts
- Features catalysts containing imine- and amine-based ligands

Contents

Fields of interest
Organic Chemistry; Polymer Sciences

Target groups
Research

Discount group
P

Due March 2011

2011. 180 p. 78 illus., 15 in color. (Springer Theses) Hardcover

$129.00
ISBN 978-3-642-18011-8

Due April 2011

2011. Approx. 250 p. 45 illus. (Catalysis by Metal Complexes, Volume 36) Hardcover

$129.00

RSCPublishing

Due January 2011

Only available in print

Distribution rights outside North and South America:
Royal Society of Chemistry, Cambridge, UK

2011. 316 p. (RSC Drug Discovery, Number 5) Hardcover

$219.00
ISBN 978-1-84973-175-4
L. Chu, Sichuan University, Chengdu, China

**Smart Membrane Materials and Systems**

*From Flat Membranes to Microcapsule Membranes*

“Smart Membrane Materials and Systems: From Flat Membranes to Microcapsule Membranes” comprehensively and systematically treats modern understanding of smart or intelligent membranes with environmental stimuli-responsive functions. The contents range from flat membranes to microcapsule membranes with various response properties, such as thermo-response, pH-response, glucose-response, molecular-recognition, and dual-/multi-stimuli-response. While chapters may be read as stand-alone, together they clearly describe design concepts, fabrication strategies and methods, microstructures and performances of smart membranes. Vivid schematics and illustrations throughout the book enhance accessibility to the technology and theories.

**Features**
- An excellent reference for designing and fabricating artificial biomimetic membranes
- The first book introducing both flat membranes and microcapsule membranes with stimuli-responsive functions
- Introducing fresh progress of smart membranes since the new century

**From the contents**

**Introduction.**

**Fields of interest**
Industrial Chemistry/Chemical Engineering; Biomaterials; Pharmaceutical Sciences/Technology

**Target groups**
Research

**Discount group**
P

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A. Grabulosa, University of Barcelona, Spain

**P-Stereogenic Ligands in Enantioselective Catalysis**

This book provides comprehensive coverage of the application of P-stereogenic ligands in homogeneous catalysis. It begins with a brief chapter on generalities of P-stereogenic compounds: history, configurational stability, and interconversions among them. The book then describes the main preparative methods, from resolution of racemates to enantioselective catalysis, before focusing on the catalytic applications of P-stereogenic ligands. Chapter 7 describes the use of the ligands in catalytic hydrogenation and related reactions whereas chapter 8 deals mainly with C-C bond forming reactions. The aim of these two final chapters is to give an outline of the usefulness of the ligands in homogeneous catalysis.

**Features**
- Provides many examples from recent primary literature
- Describes easily be able to follow the preparation methods
- Provides a single comprehensive source of information

**Contents**

Introduction.  - History of P-stereogenic compounds.  - Preparation by resolution of racemates.  - Preparation by asymmetric synthesis.  - Preparation by asymmetric catalysis.  - Interconversions between P-stereogenic compounds.  - Optical purity of P-stereogenic compounds.  - P-stereogenic ligands in reduction of double bonds.  - P-stereogenic ligands in C-C bond forming reactions.  - P-stereogenic ligands in miscellaneous reaction.

**Fields of interest**
Catalysis; Organometallic Chemistry; Chemistry/ Food Science, general

**Target groups**
Research

**Discount group**
P

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S. J. Hurst, Center for Nanoscale Materials, Argonne National Laboratory, Argonne, IL, USA (Ed.)

**Biomedical Nanotechnology**

*Methods and Protocols*

Due to their unique size-dependent properties, nanomaterials have the potential to revolutionize the detection, diagnosis, and treatment of disease by offering superior capabilities compared to conventionally-used materials. Biomedical Nanotechnology: Methods and Protocols brings together experts from a wide variety of fields to provide a practical overview of biomedical nanotechnology, from the conception of novel materials in the laboratory to the application of such structures in the clinic. After a brief introductory chapter, the first section consists of protocol chapters which provide hands-on information on the synthesis of a variety of solution-phase and surface-bound nanomaterials and their application in sensing, imaging, and/or therapeutics, while the second section consists of a series of case studies and review chapters that discuss the toxicology of nanomaterials, the regulatory pathways to US Food and Drug Administration (FDA) approval of these materials, their patenting, marketing, and commercialization, and the legal and ethical issues surrounding their use.

**Features**
- Provides versatile nanoparticle bioconjugation strategies and a comprehensive view of the use of nanomaterials in biomedicine
- Contains case studies on the translation of nanomaterials to the clinic
Includes expert tips and vital implementation advice

**Fields of interest**
Biotechnology; Nanotechnology; Biomaterials

**Target groups**
Professional/practitioner

**Discount group**
P
Sample Preparation in Biological Mass Spectrometry

The aim of this book is to provide the researcher with important sample preparation strategies in a wide variety of analyte molecules, specimens, methods, and biological applications requiring mass spectrometric analysis as a detection end-point. In this volume we have compiled the contributions from several laboratories which are employing mass spectrometry for biological analysis. With the latest inventions and introduction of highly sophisticated mass spectrometry equipment sample preparation becomes an extremely important bottleneck of biomedical analysis. We have a goal of giving the reader several successful examples of sample preparation, development and optimization, leading to the success in analytical steps and proper conclusions made at the end of the day. This book is structured as a compilation of contributed chapters ranging from protocols to research articles and reviews. The main philosophy of this volume is that sample preparation methods have to be optimized and validated for every project, for every sample type and for every downstream analytical technique.

Features
- The attention to sample preparation methods in recent years has risen considerably, both in the Academia and in the life science industry, however there are very few books on this topic.
- The book presents examples of successful optimization and validation of sample preparation for biomedical analysis.
- Latest trends in biological analysis fueled by the progress in instrument development and adoption of the latest high resolution and high sensitivity mass spectrometry methods are well covered.
- The book contains comprehensive reviews that would help the reader to acquire the most current experience in certain fields of biological sample preparation.

Fields of interest
- Analytical Chemistry
- Mass Spectrometry
- Biochemistry

Target groups
- Research

Discount group
- P

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Microwave Induced Plasma Analytical Spectrometry

This book is the most comprehensive recent publication on MIPs, consisting of 13 chapters, primarily involving the fundamentals, the instrumentation, and the methodologies of MIP-OES. The physical and chemical characteristics of the various MIP sources and sample introduction techniques available are all discussed as well as how these characteristics affect the design of the parts of the MIP setup with inclusion of some very recent work with MIP sources.

Contents
- An introduction to MIP spectrometries.
- Instrumentation for Analytical MIP spectrometry.
- Principles of operation and construction of microwave plasma cavities.
- Introduction of gases and vapours into MIP.
- Solution and slurry nebulization coupling with MIP.
- Solid sampling techniques for MIP.
- Optical emission spectrometry with MIP.
- Optimization of the MIP-OES system.
- Analytical method development.
- Analytical performance of MIP-OES.
- Analytical applications of MIP-OES.
- Non-emission MIP spectroscopic techniques.

Fields of interest
- Spectroscopy/Spectrometry
- Atomic, Molecular, Optical and Plasma Physics
- Analytical Chemistry

Target groups
- Research

Discount group
- P

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Cellulose Fibers: Bio- and Nano-Polymer Composites

Green Chemistry and Technology

Because we are living in an era of Green Science and Technology, developments in the field of bio- and nano-polymer composite materials for advanced structural and medical applications is a rapidly emerging area and the subject of scientific attention. In light of the continuously deteriorating environmental conditions, researchers all over the world have focused an enormous amount of scientific research towards bio-based materials because of their cost effectiveness, eco-friendliness and renewability. This handbook deals with cellulose fibers and nano-fibers and covers the latest advances in bio- and nano-polymer composite materials. This rapidly expanding field is generating many exciting new materials with novel properties and promises to yield advanced applications in diverse fields. This book reviews vital issues and topics and will be of interest to academicians, research scholars, polymer engineers and researchers in industries working in the subject area. It will also be a valuable resource for undergraduate and postgraduate students at institutes of plastic engineering and other technical institutes.

Features
- Summarizes state-of-the-art of cellulose fibers
- Gives applications in green technology
- Renowned international authorship

Fields of interest
- Polymer Sciences
- Environmental Chemistry
- Biomaterials

Target groups
- Research

Discount group
- P
Actinide Nanoparticle Research

This is the first book to cover actinide nanoparticle research. It is of interest both for fundamental research into the chemistry and physics of f-block elements as well as for applied researchers such as those studying the long-term safety of nuclear waste disposal and developing remediation strategies. The authors cover important issues of the formation of actinide nanoparticles, their properties and structure, environmental behavior of colloids and nanoparticles related to the safe disposal of nuclear wastes, modeling and advanced methods of characterization at the nano-scale.

Features
► First book on this topic ► Provides information for fundamental research on f-block elements ► Relevant also for nuclear waste disposal and remediation

From the contents

Fields of interest
Nuclear Chemistry; Geophysics and Environmental Physics; Geochemistry

Target groups
Research

Discount group
P

Catalytic Microreactors for Portable Power Generation

“Catalytic Microreactors for Portable Power Generation” addresses a problem of high relevance and increased complexity in energy technology. This thesis outlines an investigation into catalytic and gas-phase combustion characteristics in channel-flow platinum-coated microreactors. The emphasis of the study is on microreactor/microturbine concepts for portable power generation and the fuels of interest are methane and propane. The author carefully describes numerical and experimental techniques, providing a new insight into the complex interactions between chemical kinetics and molecular transport processes, as well as giving the first detailed report of hetero-/homogeneous chemical reaction mechanisms for catalytic propane combustion.

Features
► Nominated by the Paul Scherrer Institute for a Springer Theses Prize ► A comprehensive numerical model for the investigation of catalytic microscale reactors is used and described for the first time ► Provides valuable information of high scientific impact on the design and operation of catalytic microreactors for portable power generation.

Contents
Nomenclature Introduction Experimental setup Numerical models Experimental and numerical investigation of the hetero-/homogeneous combustion of lean propane/air mixtures over platinum Experimental and numerical investigation of a propane-fueled, catalytic, mesoscale combustor Hetero-/homogeneous combustion and stability maps in methane-fueled catalytic microreactors: channel confinement and molecular transport effects Numerical investigation on the start-up of methane-fueled, catalytic microreactors Conclusions Summary – Outlook

Fields of interest
Physical Chemistry; Power Engineering; Catalysis

Target groups
Research

Discount group
P

Chemical Kinetics with Mathcad and Maple

The authors explain at length the principles of chemical kinetics and approaches to computerized calculations in modern software suites — mathcad and maple. Mathematics is crucial in determining correlations in chemical processes and requires various numerical approaches. Often significant issues with mathematical formalizations of chemical problems arise and many kinetic problems can’t be solved without computers. Numerous problems encountered in solving kinetics’ calculations with detailed descriptions of the numerical tools are given. Special attention is given to electrochemical reactions, which fills a gap in existing texts not covering this topic in detail. The material demonstrates how these suites provide quick and precise behavior predictions for a system over time (for postulated mechanisms). Examples, i.e., oscillating and non-isothermal reactions, help explain the use of mathcad more efficiently. Also included are the results of authors’ own research toward effective computations.

Features
► Includes results from the authors’ research towards performing efficient computations ► Numerous specific types of problems that are encountered in solving kinetics calculations are discussed ► Network calculations, which do not require local installation of Mathcad are also covered ► Includes an extra section of problems for individual work ► Special attention is given to electrochemical reactions, which is normally absent in kinetic textbooks

Fields of interest
Physical Chemistry; Mathematical Software; Computer Appl. in Life Sciences

Target groups
Research

Discount group
P
**Handbook of Computational Chemistry**

The role the Handbook of Computational Chemistry is threefold. It is primarily intended to be used as a guide that navigates the user through the plethora of computational methods currently in use; it explains their limitations and advantages; and it provides various examples of their important and varied applications.

**Features**
- Handles molecular mechanics, quantum mechanics, and statistical mechanics calculations
- Provides an accessible introduction to the methods and concepts of computational and quantum chemistry
- Reviews applications in Biomolecules and Nanostructures
- Aimed at graduate students from Physics, Chemistry, Materials Science, and Biology disciplines

**Fields of interest**
Theoretical and Computational Chemistry; Nanotechnology; Computer Appl. in Life Sciences

**Target groups**
Research

**Discount group**
P

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**Computational Chemistry**

**Introduction to the Theory and Applications of Molecular and Quantum Mechanics**

This corrected second edition contains new material which includes solvent effects, the treatment of singlet diradicals, and the fundamentals of computational chemistry. “Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics” is an invaluable tool for teaching and researchers alike. The book provides an overview of the field, explains the basic underlying theory at a meaningful level that is not beyond beginners, and it gives numerous comparisons of different methods with one another and with experiment.

**Features**
- The second edition of this popular textbook takes a pedagogical approach including questions (classed as ‘harder’ and ‘easier’) which are aimed at students of varying abilities
- The only textbook on this subject to genuinely cover the basics
- Each chapter is presented with an initial historical overview thus enlightening students and guiding them away from the usual ‘dry’ presentation of facts
- A must for computational chemistry university lecturers

**Contents**
1. An outline of what computational chemistry is all about.
2. The concept of the potential energy surface.
4. Introduction to quantum mechanics in computational chemistry.
5. Ab initio calculations.
8. Some “special” topics: (a) solvation, (b) singlet diradicals, (c) a note on heavy atoms and transition metals.
9. Selected literature highlights, books, websites, software and hardware.

**Fields of interest**
Theoretical and Computational Chemistry; Computer Applications in Chemistry; Organic Chemistry

**Target groups**
Graduate

**Discount group**
P

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**High Performance Chelation Ion Chromatography**

The book describes the underlying principles which give rise to the special selectivities that can be chosen for separating specific groups of metals. It also covers the latest research and gives many examples of its application to real samples. The very latest developments in detection techniques are included showing that HPCIC can rival atomic spectroscopic techniques such as ICP-MS. The detailed description of the fundamental principles controlling the separation of trace metals using chelating substrates is unique to this book. It shows how HPCIC differs from the commonly used simple ion exchange techniques and how these chelation characteristics give rise to a much more useful and versatile metal separation system. Readers will also be interested in the analysis of extremely difficult matrices, such as saturated brines, easily achieved by HPCIC but requiring extremely difficult matrices, such as saturated brines, easily achieved by HPCIC but requiring very complex multi column systems using other ion chromatography methods.

**Features**
- Written by experts
- Up-to-date
- Presents a comprehensive survey of the field

**Contents**
Introduction.- Separation Mechanisms.- Chelating stationary phases.- Eluents for HPCIC.- Chelating parameters and influence of chelation and ion exchange on the retention and separation of metal ions.- Detection.- Applicability of HPCIC to analysis.- Conclusions.

**Fields of interest**
Chromatography

**Target groups**
Research

**Discount group**
P

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**Due October 2011**

In 4 volumes, not available separately.

2011. 1600 p. Hardcover

**Due May 2011**


2nd ed. 2011. XVI, 664 p. Softcover

**Due January 2011**

Only available in print

Distribution rights outside North and South America: Royal Society of Chemistry, Cambridge, UK


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Challenges in Analytical Quality Assurance

Working in the lab, but unsure what your results actually mean? Would you like to know how to apply trueness tests, calculate standard deviations, estimate measurement uncertainties or test for linearity? This book offers you a problem-based approach to analytical quality assurance (AQA). After a short introduction into required fundamentals, various topics such as statistical tests, linear regression and calibration, tool qualification or method validation are presented in the form of exercises for self-study. Solutions are provided in a clear step-by-step manner. Interactive Excel-sheets are available as Extra Materials for trying out the various concepts. For professionals as well as graduate students confronted with analytical quality assurance for the first time, this book will be the clue to meeting such challenges.

Features
► Problem-based learning of the principles of Analytical Quality Assurance
► Excel-sheets for interactive self-study available as Extra Materials
► From the authors of popular Analytical Challenges in the journal Analytical and Bioanalytical Chemistry

Contents

Fields of interest
Analytical Chemistry; Monitoring/Environmental Analysis; Pharmaceutical Sciences/Technology

Target groups
Professional/practitioner

Discount group
P

Biodegradable Poly (Lactic Acid)
Synthesis, Modification, Processing and Applications

“Biodegradable Poly (Lactic Acid): Synthesis, Modification, Processing and Applications” describes the preparation, modification, processing, and the research and applications of biodegradable poly (lactic acid), which belong to the biomedical and environment-friendly materials. Highly illustrated, the book introduces systematically the synthesis, physical and chemical modifications, and the latest developments of research and applications of poly (lactic acid) in biomedical materials. The book is intended for researchers and graduate students in the fields of materials science and engineering, polymer science and engineering, biomedicine, chemistry, environmental sciences, textile science and engineering, package materials, and so on. Dr. Jie Ren is a professor at the Institute of Nano and Bio-Polymeric Materials, School of Material Science and Engineering, Tongji University, Shanghai, China.

Features
► Discusses novel biodegradable materials and applications in a highly evolving market
► First book to systematically introduce poly (lactic acids)
► Describes wide applications from biomaterials to environmental packaging
► Highly illustrated

Contents
Introduction.- Raw materials.- Synthesis and manufacture of poly (lactic acid).- Modification of poly (lactic acid).- Processing of poly (lactic acid).- Application in the field of commodity and industry product.- Application in the field of biomedical materials.- Standard and Test Methods.

Fields of interest
Polymer Sciences; Biochemical Engineering; Waste Management/Waste Technology

Target groups
Research

Discount group
P

Due March 2011

Distribution rights in China: Tsinghua University Press.

Jointly published with Tsinghua University Press

Topics in Current Chemistry

Volume 299

H. Nagase, School of Pharmacy, Kitasato University, Tokyo, Japan (Ed.)

Chemistry of Opioids

Features
► This series presents critical reviews of the present position and future trends in modern chemical research
► Short and concise reports on chemistry, each written by the world renowned experts
► Still valid and useful after 5 or 10 years
► More information as well as the electronic version of the whole content available at: springerlink.com

Contents

Fields of interest
Biorganic Chemistry; Animal Biochemistry; Molecular Medicine

Target groups
Research

Discount group
P

Due March 2011

► $349.00
ISBN 978-3-642-18106-1

Due January 2011

2011. 333 p. 100 illus. Hardcover
► $129.00
ISBN 978-3-642-16594-8

2011. 240 p. 120 illus. Hardcover
► $169.00
ISBN 978-3-642-17595-4
Topics in Organometallic Chemistry

Volume 35
A. J. Canty (Ed.)

Higher Oxidation State Organopalladium and Platinum Chemistry


Features
- Each volume of Topics in Organometallic Chemistry provides the broad scientific reader with a comprehensive and critical overview of a specific topic in organometallic chemistry
- Research in this rapidly developing transdisciplinary field is having profound influence on other areas of scientific investigation, ranging from catalytic organic synthesis to biology, medicine and material science

Fields of interest
Organometallic Chemistry; Catalysis; Organic Chemistry

Target groups
Research

Discount group
P

Functional Molecules from Natural Sources

Written by leading industrial and academic practitioners from each sector, the book offers authoritative updates on new approaches to the use of naturally occurring compounds within the pharmaceutical, nutraceutical and agrochemical industries. Several case studies on important natural product leads, or functional molecules, are presented with the strategy for their development. These new medical applications in the use of familiar natural molecules and advances in the understanding and manipulation of natural product biosynthesis at the genetic level. Highlights include an authoritative review of the entire field of natural anticancer agents emphasizing those currently in clinical development, an account of the optimization of the pleuromutilin antibiotic template for human use and a comprehensive description of the research programme that resulted in the discovery of platensimycin.

Features
- Provides a unique source of information
- Highlights current trends
- Presented by recognised leaders in the subject area

Contents
Modern and Emerging Perspectives on Natural Product Utilisation.- Improved Strategies for Natural Product Exploitation.- Functional Molecules and Their Enhancement.- Biosynthesis and Genetics.- Summary of Other Lectures.

Fields of interest
Organic Chemistry; Biotechnology; Pharmaceutical Sciences/Technology

Target groups
Research

Discount group
P

Linear-Scaling Techniques in Computational Chemistry and Physics

“Linear-Scaling Techniques in Computational Chemistry and Physics“ summarizes recent progresses in linear-scaling techniques and their applications in chemistry and physics. In order to meet the needs of a broad community of chemists and physicists, the book focuses on recent advances that extended the scope of possible exploitations of the theory.

Features
- The only handbook to present a comprehensive overview of linear-scaling methods and their applications
- Incorporates the very latest developments in the field
- Applications aimed at those working in computational chemistry and physics

From the contents

Fields of interest
Theoretical and Computational Chemistry; Theoretical, Mathematical and Computational Physics

Target groups
Research

Discount group
P

Due March 2011

RSCPublishing

Due January 2011

Only available in print

Distribution rights outside North and South America:
Royal Society of Chemistry, Cambridge, UK

2011. 400 p. 120 Illus., 89 in color. (Challenges and Advances in Computational Chemistry and Physics, Volume 13) Hardcover

approx. $369.00