Computational Studies of Transition Metal Nanoalloys

The focus of this thesis is the computational modelling of transition metal bimetallic (nano-alloy) clusters. More specifically, the study of Pd-Pt, Ag-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 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.

Contents

Fields of interest
Theoretical and Computational Chemistry; Nanoscience; Catalysis

Target groups
Research

Type of publication
Monograph

Due March 2011

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

- € 99,95 | £90.00
- - (D) 106,95 € (A) 109,95 | sFr 143,50
ISBN 978-3-642-18011-8

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

Type of publication
Monograph

Due February 2011

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

- € 99,95 | £90.00
- - (D) 106,95 € (A) 109,95 | sFr 143,50
ISBN 978-3-642-18011-8

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 functionalities. 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 cover design concepts, fabrication strategies and methods, microstructures and performances of smart membranes. Vivid schematics and illustrations throughout the book enhance accessibility to the theory and technologies.

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

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

Target groups
Research

Type of publication
Monograph
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

Type of publication
Contributed volume

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, 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, general

Target groups
Research

Type of publication
Contributed volume

Due March 2011

11. 415 p. 104 illus., 11 in color. (Methods in Molecular Biology, Volume 726) Hardcover

- € 109.95 | £99.00
- * € (D) 117.65 | € (A) 120.95 | sFr 158.00

Due April 2011

11. X. 690 p. 225 illus., 75 in color. Hardcover

- € 169.95 | £153.00
- * € (D) 181.85 | € (A) 186.94 | sFr 244.00
ISBN 978-1-61779-075-1

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 cellulose fibers
- Gives applications in green technology
- Renowned international authorship

Fields of interest
Polymer Sciences; Environmental Chemistry; Biomaterials

Target groups
Research

Type of publication
Monograph

Due March 2011

11. 750 p. Hardcover

- € 239.00 | £215.50
- * € (D) 255.73 | € (A) 262.90 | sFr 343.00
ISBN 978-3-642-17369-1
Actinide Nanoparticle Research

This is the first book to cover actinide nano 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 nano-particles, 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

Type of publication
Monograph

Due February 2011

2011. 388 p. 204 illus. Hardcover
▶ approx. € 139,95 / £126.00
▶ approx. € (D) 149,75 / € (A) 153,94 / sFr 201,00
ISBN 978-3-642-11431-1

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/micro-turbine 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

Fields of interest
Physical Chemistry; Power Engineering; Catalysis

Target groups
Research

Type of publication
Monograph

Due January 2011

2011. 110 p. 59 illus., 13 in color. (Springer Theses) Hardcover
▶ € 99,95 / £90.00
▶ approx. € (D) 106,95 / € (A) 109,95 / sFr 143,50
ISBN 978-3-642-11667-4

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

Type of publication
Monograph

Due April 2011

2011. 400 p. 230 illus. Hardcover
▶ approx. € 139,95 / £126.00
▶ approx. € (D) 149,75 / € (A) 153,94 / sFr 201,00
ISBN 978-3-7091-0530-6
J. Leszczynski, Jackson State University, Jackson, MS, USA (Ed.)

**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, Material Science, and Biology disciplines

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

**Target groups**
Research

**Type of publication**
Handbook

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E. G. Lewars, Trent University, Peterborough, ON, Canada

**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. It includes 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**

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M. Reichenbächer, J. W. Einax, University of Jena, Germany

**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

**Type of publication**
Professional book

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Due January 2011

In 4 volumes, not available separately.

2011. 1600 p. Hardcover
- approx. € 699,00 | £629.50
- approx. *€ (D) 787,92 | € (A) 768,90 | sFr 1002,50 ISBN 978-94-007-0711-3

2011. 1600 p. eReference
- approx. € 699,00 | € 629.50
- approx. *€ (D) 831,81 | € (A) 838,80 | sFr 1053,00 ISBN 978-94-007-0711-3

2011. 1600 p. Print + eReference
- approx. € 874,00 | £787.00
- approx. *€ (D) 935,10 | € (A) 961,40 | sFr 1253,00 ISBN 978-94-007-0711-3

Due April 2011


2nd ed. 2011. XVI, 664 p. Softcover
- approx. € 75,00 | £68.99
- approx. *€ (D) 80,25 | € (A) 82,50 | sFr 108,00 ISBN 978-90-481-3861-4

Due January 2011

2011. 333 p. 100 Illus. Hardcover
- € 99,95 | £90.00
- *€ (D) 106,95 | € (A) 109,95 | sFr 143,50 ISBN 978-3-642-16594-8
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-Polymer 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


Fields of interest

Polymer Sciences; Biochemical Engineering; Waste Management/Waste Technology

Target groups

Research

Type of publication

Monograph

Due February 2011

Distribution rights in China: Tsinghua University Press.

Jointly published with Tsinghua University Press

2011. 240 p. 120 Illus. Hardcover

€ 119,95 | £108.00

ISBN 978-3-642-18106-1
Linear-Scaling Techniques in Computational Chemistry and Physics

Methods and Applications

“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

Type of publication
Monograph

Due March 2011

2011. 400 p. 120 illus., 89 in color. (Challenges and Advances in Computational Chemistry and Physics, Volume 13) Hardcover
★ approx. € 299,00
★ approx. ** € (D) 319,93 | € (A) 328,90