

Time-Dependent Density Functional Theory. From the series: Lecture Notes in Physics, Volume 706.

Edited by Miguel A. L. Marques (Universidade de Coimbra, Portugal), Carsten A. Ullrich (University of Missouri-Columbia, MO), Fernando Nogueira (Universidade de Coimbra), Angel Rubio (Universidad del País Vasco, San Sebastián, Spain), Kieron Burke (Rutgers University, Piscataway, NJ), and Eberhard K. U. Gross (Freie Universität, Berlin, Germany). Springer: Berlin, Heidelberg, New York. 2006. xxxiv + 590 pp. \$99.00. ISBN 3-540-35422-0.

Recent years have been marked by important formal and practical developments in time-dependent density functional theory (TD-DFT), which extends ground-state DFT to time-dependent processes, excited states, and response properties. This book offers a discussion of the underlying ideas and theorems of TD-DFT, which are distinct from the ground-state DFT and provides a conceptual framework for the theory and coverage of its implementation. Ample space is dedicated to applications, and a glimpse of current frontiers is also provided.

Time-Dependent Density Functional Theory represents a concise overview of the field and thus is long overdue. Unlike many reviews, this is a well-structured text, with a common set of notations and a single comprehensive and up-to-date list of references, rather than just a compilation of research articles. Because of its clear organization, the book can be used by novices (basic knowledge of ground-state DFT is assumed) and experienced users of TD-DFT, as well as developers in the field. Selected chapters can be used as an instructor's resource in classes on advanced electronic structure. The extensive set of applications demonstrates the strength and limitations of TD-DFT and nicely complements more formal material.

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Frontiers in Transition Metal-Containing Polymers.

Edited by Alaa S. Abd-El-Aziz (University of British Columbia Okanagan, Kelowna, Canada) and Ian Manners (University of Bristol, U.K.). John Wiley & Sons, Inc.: Hoboken, NJ. 2007. x + 534 pp. \$135. ISBN: 0-471-73015-7.

This book is a very thorough review of the latest trends in metallopolymer research. To fully appreciate the extent of this work the reader should have a good knowledge of polymer chemistry, especially basic terminology, which is not covered. Each chapter is comprehensively referenced, however, directing the reader who is not familiar with this area of chemistry to articles or reviews that cover these basic concepts in detail.

The first two chapters outline general information pertaining to the development of this broad field of research. Starting with

the discovery of the first organometallic polymer in 1955, the authors of the first chapter describe over 100 structures that were prepared in the ensuing five decades. The second chapter is a more focused review of the research done in this field since 1990. As expected, Chapter 1 has a few pivotal references that are 20 or 30 years old; the remaining citations are recent and primarily from the past decade. These introductory chapters effectively put the remainder of the book into context while also highlighting the importance of the field.

Chapters 3–7 thoroughly outline the synthesis and properties of a variety of metal-containing polymers while also pointing out the many applications envisioned for these materials. A very significant description of the use of these polymers in nanofabrication is presented in Chapter 5. This kind of review is essential due to the major developments in this nascent field. The content of the other chapters is diverse; it ranges from extensive discussion on spectroscopic characteristics to detailed descriptions of the synthetic protocols for preparing metal-containing polymers. This section is clearly of interest to researchers who focus on the synthesis and properties that metallopolymer possess; the authors also identify many unique properties that arise from incorporating metals into the backbone or side chains.

The final six chapters concentrate on the versatility of metal-containing polymers. The authors successfully accomplish this by focusing on the interdisciplinary nature of this research and by giving emphasis to the many applications of these macromolecules. Chapter 8 is an in-depth review of the recent developments of 1-D metallopolymer and oligomers; over 70% of the references in this chapter are from 2000 or later. Chapter 9 is a discussion of multiredox systems that arise from redox functionalities in polymers. These systems are of interest in the area of solid-state memory. Following this section, Chapter 10 focuses on dendrimers made from different transition metals and the catalytic properties of these macromolecules as well as their applications. Chapter 11 concentrates on metal dendritic iron polymers and their uses, whereas the last two chapters may be of interest to chemical biologists. More specifically, Chapter 12 covers iron-containing metallobiopolymers and features the extensive use of crystal structures to convey important properties of these molecules. The last chapter deals with supramolecular architectures containing metals. Their organization is centered on modified DNA bases that bind to metals to provide well-defined structures. In our opinion, Chapter 5, "Metal Coordination Polymers for Nanofabrication", would have been better placed among these final chapters because it also covers such concepts as self-assembly and surface chemistry. However, this is just a personal preference and should not be taken as a negative aspect of the book.

In summary, this book is a recent review of topical research in metal-containing polymers. Previous work in this area and the importance of these macromolecules are emphasized in the early chapters followed by an exhaustive review on the synthesis of different metallopolymer and discussions of how metal incorporation results in unique properties. Finally, the book

covers polymers that have potential applications in chemistry, computers, and biomedicine. This book is highly recommended for researchers with previous knowledge on the field of polymer chemistry.

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Nanocatalysis. Edited by Ulrich Heiz (Technische Universität München, Germany) and Uzi Landman (Georgia Institute of Technology, Atlanta, GA). From the series: Nanoscience and Technology. Edited by P. Avouris, B. Bhushan, D. Bimberg, K. von Klitzing, H. Sakaki, and R. Wiesendanger. Springer: Berlin, Heidelberg, New York. 2007. xvi + 504 pp. \$179.00. ISBN 978-3-540-32645-8.

This book is one in the series *Nanoscience and Technology* by Springer. It should be useful to chemists, chemical engineers, and materials scientists entering the field of nanocatalysts as well as to experts already in the area. Major aspects covered include nanosize metal clusters both as is and supported, lithography in nanocatalysis, and films of nano-oxides of late transition metals. Major emphasis is placed on gold clusters throughout the book.

The book was written to emphasize current methodologies and pedagogies, including basic research and catalytic applications. Both experimental and fundamental aspects are covered, and thorough introductions are included. Size-dependent properties are a recurring theme throughout the book. In general, the book progresses from the smallest clusters, having tens of atoms, to the largest, having thousands. Detailed discussions of ways to generate clusters; detection via mass spectrometry, photoelectron spectroscopy, and vibrational spectroscopy; electron diffraction; electron energy-loss spectroscopy; X-ray absorption; scanning tunneling microscopy; thermal desorption; thermal reaction; and absorption methods are provided. Excellent descriptions of density functional theory and first principles molecular dynamics are given. Theories of catalysis and catalytic mechanisms are summarized with respect to catalytic activation of CO oxidation. Fundamental concepts of spillover, electronic effects, geometric effects, cooperative adsorption, and fluxionality are also introduced. Besides Au, clusters of Pt and Pd are discussed.

Considerable discussion of MgO clusters is also given, and the role of point defects is introduced. Low-coordinated cations and anions, hydroxyl groups, anion and cation vacancies, divacancies, impurity atoms, *O*-radicals, anion vacancy aggregates, shallow and deep electron traps, and microfacets are covered. An excellent discussion is provided of how to characterize these defect sites and their importance in catalytic reactions. Deposition of metal atoms on such defect sites is also discussed.

Catalysis by nanoparticles is a large part of the book. The emphasis here is on the role of nanosize particles in a catalytic reaction. Support and morphology effects, electronic band structure, and properties of the catalyst are discussed.

Nanofabrication and nanolithography of nanosize materials is the focus of one of the six major chapters. Generation of

lithographic materials with *in situ* vapor deposition, spin coating, self-assembly routes, electron beam methods, and colloidal methods are discussed. Catalysis of oxidation via thin films and bulk metal oxides is primarily related to CO oxidations. Naked gold, gold single crystals, and colloidal gold in various processes, including CO oxidation, water gas shift reactions, vinyl acetate syntheses, hydrochlorination of ethyne, selective oxidations, epoxidations, hydrogenations, formation of hydrogen peroxide, NO_x reduction, oxidative decomposition of dioxins and volatile organic compounds, hydrocarbon combustion, ozone decomposition, SO₂ removal, Heck reactions, activation of CO₂, and other reactions catalyzed by gold species are thoroughly reviewed as is their resistance to sulfur poisoning. Potential industrial applications, such as in fuel cells, sensors, air cleaning, and autocatalysts, are presented.

This book is of considerable importance to the chemical community. All chapters are well written and illustrated and contain essential introductory as well as detailed reference information. The references are almost all from the past 5 years or so and summarize recent developments in this area. In particular, those studying catalysis over gold catalysis will find this book very thorough. The backgrounds of most of the authors are in physics and chemistry. Theoretical aspects of this field are thus well explained and understandable.

The scope of the book concerns synthesis, characterization, theoretical ideas, and applications of small metal clusters. The book fulfills its objectives of serving as an introductory text for the field of nanocatalysis as well as offering excellent summaries of current state-of-the-art problems and approaches available to make, characterize, and use such nanosize materials.

In summary, this book on the whole is an excellent contribution. It could be used as a textbook, reference, and starting point for other books in this series. It is easy to read and well organized as well as contains a significant number of graphics of all types.

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Calixarenes in the Nanoworld. Edited by Jacques Vicens (ECPM-ULP-CERNS, Strasbourg, France) and Jack Harrowfield (ISIS-ULP-CERNS, Strasbourg, France). Assistant Editor: Lassaad Baklouti (FSB, Bizerte, Tunisia). Springer: Dordrecht. 2007. x + 396 pp. \$189.00. ISBN 1-40205-021-6.

The title of this book aptly describes its contents and the prominent role that calixarenes have played in the rapid development of nanotechnology and material science over the past few years. The editors and authors of the chapters are clearly recognized as leaders in the chemistry of calixarenes based on their sustained and innovative contributions to the field. In addition, the large number of contemporary and relevant citations to the literature makes this a helpful reference book.

Calixarenes in the Nanoworld is different from most of the previous tomes addressing the chemistry of calixarenes in that it focuses more on their molecular-level processes and functions and less on their structure and conformation. Besides emphasizing the traditional biomimetic applications of calixarenes as host

molecules and catalysts, the book also highlights the emerging frontiers in which their supramolecular properties and architectural features are exploited in sensors, nanoscale machines, and novel materials. For those who are new to calixarenes, the book will provide a compelling view of the vast landscape that calixarenes encompass, and for those who have worked in the field for some time, it is an entertaining compendium of the incremental advances that have resulted in calixarenes as a main stay in the nanoworld. Overall, the book will inspire scientists in many disciplines to explore the wondrous potential of this versatile family of molecules.

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Advances in Biopolymers: Molecules, Clusters, Networks, and Interactions. ACS Symposium Series 935. Edited by Marshall L. Fishman (U.S. Department of Agriculture), Phoebe X. Qi (U.S. Department of Agriculture), and Louise Wicker (University of Georgia). American Chemical Society: Washington, DC (distributed by Oxford University Press). 2006. xii + 316 pp. \$179.50. ISBN 0-8412-3959-2.

This book was developed from a symposium on the titled subject held at the 228th American Chemical Society National Meeting in Philadelphia, PA in August 2004. It begins with two overview chapters: “New Views of Protein Structures: Implications for Potential New Protein Structure—Function Relationships: Protein Structure and Functionality” and “Polysaccharides: Molecules, Clusters, Networks, and Interactions”. The remaining 18 chapters are organized into the

following thematic sections: Protein Structure and Function; Polysaccharides Structure and Function; and Novel Approaches of Biopolymers. An author and a subject index complete the book.

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Multifunctional Conducting Molecular Materials. Edited by Gunzi Saito (Kyoto University, Japan), Fred Wudl (University of California, Los Angeles, USA), Robert C. Haddon (University of California, Riverside, USA), Katsumi Tanigaki (Tohoku University, Miyagi, Japan), Toshiaki Enoki (Tokyo Institute of Technology, Japan), Howard E. Katz (Johns Hopkins University, Baltimore, USA), Mitsuhiro Maesato (Kyoto University). Royal Society of Chemistry: Cambridge. 2007. xii + 305 pp. \$189.00. ISBN 0-85404-496-5.

This book was developed from the symposium “Science and Engineering of the Future with Multifunctional Conducting Molecular Materials” held at the 2005 International Chemical Congress of the Pacific Basin Societies in Honolulu, HI in December 2005. Its 54 chapters are organized under the following headings: Molecular Conductors and Superconductors; Design and Synthesis of Functional Molecular Materials; Organic/Inorganic Hybrids and Photoinduced Phenomena; Fullerenes, Nanotubes and Other Related Nano Materials; and Integration and Functionalities of Molecular Materials. A brief subject index completes the book.

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