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Springer

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**Jon A. McCleverty, Thomas J. Meyer**



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*Principles and Applications of Density Functional Theory in Inorganic Chemistry II* Nikolas Kaltsoyannis, John E. McGrady, 2004. E. Clot, O. Eisenstein, Agostic Interactions from a Computational Perspective. One Name, many Interpretations. Robert J. Deet, Recent Developments in Computational Bioinorganic Chemistry. E. Ruiz, Theoretical Study of the Exchange Coupling in Large Polynuclear Transition Metal Complexes Using DFT Methods. D. Snchez Portal, P. Ordejón, E. Canadell, Computing the Properties of Materials from First Principles with SIESTA. F. Cor M. Alfredsson, G. Mallia, D. S. Middlemiss, W. C. Mackrodt, R. Dovesi, R. Orlando, The Performance of Hybrid Density Functionals in Solid State Chemistry.

**Crystal Engineering: From Molecules and Crystals to Materials** Dario Braga, Fabrizia Grepioni, A. Guy Orpen, 2012-12-06. Crystal engineering is an interdisciplinary area that cuts across the traditional subdivisions of chemistry. Fuelled by our increasingly precise understanding of the chemistry and properties of supramolecular systems, interest in the potential of the field has increased rapidly. The topics discussed in the 28 contributions in this book provide a state-of-the-art description of the field and offer new research ideas that if pursued will serve to strengthen the field at the interface between supramolecular chemistry and materials science.

Iodine Catalysis in Organic Synthesis Kazuaki Ishihara, Kilian Muniz, 2022-01-10. Iodine Catalysis in Organic Synthesis. The first book of its kind to highlight iodine as a sustainable alternative to conventional transition metal catalysis. Iodine Catalysis in Organic Synthesis provides detailed coverage of recent advances in iodine chemistry and catalysis, focusing on the utilization of various iodine-containing compounds as oxidative catalysts. Featuring contributions by an international panel of leading research chemists, this authoritative volume explores the development of environmentally benign organic reactions and summarizes catalytic transformations of molecular iodine and iodine compounds such as hypervalent organoiodine and inorganic iodine salts. Readers are first introduced to the history of iodine chemistry, the conceptual background of homogeneous catalysis, and the benefits of iodine catalysis in comparison with transition metals. Next, chapters organized by reaction type examine enantioselective transformations, catalytic reactions involving iodine catalyst states, oxidation in iodine, and iodine catalyses and catalytic reactions based on halogen bonding. Practical case studies and real-world examples of different applications in organic synthesis and industry are incorporated throughout the text. An invaluable guide for synthetic chemists in both academic and industrial laboratories. Iodine Catalysis in Organic Synthesis provides a thorough overview of typical iodine-catalyzed reactions, catalyst systems, structures, and reactivity. Explores promising industrial applications of iodine-based reagents for organic synthesis. Highlights the advantages iodine catalysis has over classical metal-catalyzed reactions. Discusses sustainable and eco-friendly methods in hypervalent iodine chemistry. Edited by two world authorities on the

catalytic applications of organoiodine compounds Iodine Catalysis in Organic Synthesis is required reading for catalytic organic and organometallic chemists medicinal and pharmaceutical chemists industrial chemists and academic researchers and advanced students in relevant fields      Self-healing Materials Martin D. Hager, Sybrand van der Zwaag, Ulrich S. Schubert, 2016-07-06 The series Advances in Polymer Science presents critical reviews of the present and future trends in polymer and biopolymer science It covers all areas of research in polymer and biopolymer science including chemistry physical chemistry physics material science The thematic volumes are addressed to scientists whether at universities or in industry who wish to keep abreast of the important advances in the covered topics Advances in Polymer Science enjoys a longstanding tradition and good reputation in its community Each volume is dedicated to a current topic and each review critically surveys one aspect of that topic to place it within the context of the volume The volumes typically summarize the significant developments of the last 5 to 10 years and discuss them critically presenting selected examples explaining and illustrating the important principles and bringing together many important references of primary literature On that basis future research directions in the area can be discussed Advances in Polymer Science volumes thus are important references for every polymer scientist as well as for other scientists interested in polymer science as an introduction to a neighboring field or as a compilation of detailed information for the specialist Review articles for the individual volumes are invited by the volume editors Single contributions can be specially commissioned Readership Polymer scientists or scientists in related fields interested in polymer and biopolymer science at universities or in industry graduate students      *Principles and Applications of Density Functional Theory in Inorganic Chemistry I* Nikolas Kaltsoyannis, John E. McGrady, 2004-09-14 It is difficult to overestimate the impact that density functional theory has had on computational quantum chemistry over the last two decades Indeed this period has seen it grow from little more than a theoretical curiosity to become a central tool in the computational chemist's armoury Arguably no area of chemistry has benefited more from the meteoric rise in density functional theory than inorganic chemistry the ability to obtain reliable results in feasible time scales on systems containing heavy elements such as the d and f transition metals has led to an enormous growth in computational inorganic chemistry The inorganic chemical literature reflects this growth it is almost impossible to open a modern inorganic chemistry journal without finding several papers devoted exclusively or in part to density functional theory calculations The real importance of the rise in density functional theory in inorganic chemistry is undoubtedly the much closer synergy between theory and experiment than was previously possible In these volumes world leading researchers describe recent developments in the density functional theory and its applications in modern inorganic and bioinorganic chemistry These articles address key issues key issues in both solid state and molecular inorganic chemistry such as spectroscopy mechanisms catalysis bonding and magnetism The articles in volume I are more focussed on advances in density functional methodology while those in Volume II deal more with applications although this is by no means a rigid distinction      **Photoactive Functional Soft Materials** Quan

Li,2019-04-29 This book covers the design synthesis properties and applications of functional photoactive soft materials including aspects of polymers block copolymers elastomers biomaterials liquid crystals chemical and physical gels colloids and host guest systems It combines in a unified manner authoritative accounts describing various structural and functional aspects of photoactive soft materials Photoactive Functional Soft Materials Preparation Properties and Applications Brings together the state of the art knowledge on photoactive functional soft materials in a unified manner Covers a vibrant research field with tremendous application potential in areas such as optoelectronics photonics and energy generation Appeals to a large interdisciplinary audience because it is highly useful for researchers and engineers working on photonics optoelectronics imaging and sensing nanotechnology and energy materials Photoactive Functional Soft Materials Preparation Properties and Applications focuses on the design and fabrication of photoactive functional soft materials for materials science nanophotonics nanotechnology and biomedical applications **Click Chemistry for Biotechnology and**

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cross fertilization of physico chemical and mathematical ideas has a long historical tradition This volume of Advances in Chemical Engineering is almost completely dedicated to a conference on Mathematics in Chemical Kinetics and Engineering MaCKiE 2007 which was held in Houston in February 2007 bringing together about 40 mathematicians chemists and chemical engineers from 10 countries to discuss the application and development of mathematical tools in their respective fields Updates and informs the reader on the latest research findings using original reviews Written by leading industry experts and scholars Reviews and analyzes developments in the field **Comprehensive Coordination Chemistry II** Jon A. McCleverty,Thomas J. Meyer,2004

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