



THEORETICAL AND COMPUTATIONAL CHEMISTRY 16



Computational Photochemistry

Massimo Olivucci
editor

Computational Photochemistry

Massimo Olivucci



Computational Photochemistry:

Computational Photochemistry Massimo Olivucci, 2005-10-20 Computational Photochemistry Volume 16 provides an overview of general strategies currently used to investigate photochemical processes Whilst contributing to establishing a branch of computational chemistry that deals with the properties and reactivity of photoexcited molecules the book also provides insight into the conceptual and methodological research lines in computational photochemistry Packed with examples of applications of modelling of basic photochemical reactions and the computer aided development of novel materials in the field of photodegradation paints photoprotection sunscreens color regulation photochromic devices and fluorescent probes this book is particularly useful to anyone interested in the effect of light on molecules and materials Provides an overview of computational photochemistry dealing with principles and applications Demonstrates techniques that can be used in the computer aided design of novel photo responsive materials Written by experts in computational photochemistry

Theoretical and Computational Photochemistry García Iriepa Cristina, Marco Marazzi, 2023-04-21 Theoretical and Computational Photochemistry Fundamentals Methods Applications and Synergy with Experimental Approaches provides a comprehensive overview of photoactive systems and photochemical processes After an introduction to photochemistry the book discusses the key computational chemistry methods applied to the study of light induced processes over the past decade and further outlines recent research topics to which these methods have been applied By discussing the synergy between experimental and computational data the book highlights how theoretical studies could facilitate understanding experimental findings This helpful guide is for both theoretical chemists and experimental photochemistry researchers interested in utilizing computational photochemistry methods for their own work Reviews the fundamentals of photochemistry helping those new to the field in understanding key concepts Provides detailed guidance and comparison of computational and theoretical methods highlighting the suitability of each method for different case studies Outlines current applications to encourage discussion of the synergy between experimental and computational data and inspiring further application of these methods to other photochemical processes

Computational Methods in Photochemistry Andrei G. Kutateladze, 2005-05-05 Addressing critical aspects of computational modeling in photochemistry Molecular Methods in Photochemistry is designed to familiarize researchers and practitioners with state of the art computational methods to predict the reactivity of excited molecules It provides practical guidelines and examples for the modeling of excited states and describ

Computational Photocatalysis Dmitri Kilin, Svetlana Kilina, Yulun Han, 2021-02 Photochemical reactions and the underlying photophysical principles play key roles in the rational design of efficient systems for energy conversion and storage This volume on interfaces contains fundamental theory computational models and applications for real materials Edited by experts with a deep knowledge of the community the volume will be useful to computational chemists materials scientists physical chemists and especially those working in energy and nanomaterials

Heterogeneous Gold Catalysts and

Catalysis Zhen Ma, Sheng Dai, 2014-09-10 Once considered an inert element gold has recently gained attention as a catalyst With hundreds of papers being published each year this book presents a comprehensive review of this rapidly evolving field with contributions by leading experts across the globe Going through the chapters citing the primary literature the reader will gain a thorough background to the use of gold in catalysis as well as the latest methods for the preparation of gold catalysts Other chapters demonstrate the characterisation and modelling of gold catalysed reactions with consideration given to both the fundamentals and commercial applications of this emerging group of catalysts Written to be accessible by postgraduates and newcomers to the field this book will also benefit experienced researchers and therefore be an essential reference in the laboratory

Electron Paramagnetic Resonance Bruce Gilbert, Damien M Murphy, Victor Chechik, 2014-09-30 The topics covered in this series describe contrasting types of Electron Paramagnetic Resonance EPR application with results being set into the context of earlier work and presented as a set of critical yet coherent overviews

Multi-scale Quantum Models for Biocatalysis Darrin M. York, Tai-Sung Lee, 2009-05-30 Multi scale Quantum Models for Biocatalysis explores various molecular modelling techniques and their applications in providing an understanding of the detailed mechanisms at play during biocatalysis in enzyme and ribozyme systems These areas are reviewed by an international team of experts in theoretical computational chemistry and biophysics This book presents detailed reviews concerning the development of various techniques including ab initio molecular dynamics density functional theory combined QM MM methods solvation models force field methods and free energy estimation techniques as well as successful applications of multi scale methods in the biocatalysis systems including several protein enzymes and ribozymes This book is an excellent source of information for research professionals involved in computational chemistry and physics material science nanotechnology rational drug design and molecular biology and for students exposed to these research areas

Contemporary Carbene Chemistry Robert A. Moss, Michael P. Doyle, 2013-11-25 Presents the most innovative results in carbene chemistry setting the foundation for new discoveries and applications The discovery of stable carbenes has reinvigorated carbene chemistry research with investigators seeking to develop carbenes into new useful catalysts and ligands Presenting the most innovative and promising areas of carbene research over the past decade this book explores newly discovered structural catalytic and organometallic aspects of carbene chemistry with an emphasis on new and emerging synthetic applications Contemporary Carbene Chemistry features contributions from an international team of pioneering carbene chemistry researchers Collectively these authors have highlighted the most interesting and promising areas of investigation in the field The book is divided into two parts Part 1 Properties and Reactions of Carbenes explores new findings on carbene stability acid base behavior and catalysis Carbenic structure and reactivity are examined in chapters dedicated to stable carbenes carbodicarbenes carbenes as guests in supramolecular hosts tunneling in carbene and oxacarbene reactions and ultrafast kinetics of carbenes and their excited state precursors Theoretical concerns are

addressed in chapters on computational methods and dynamics applied to carbene reactions Part 2 Metal Carbenes is dedicated to the synthetic dimensions of carbenes particularly the reactions and catalytic properties of metal carbenes The authors discuss lithium rhodium ruthenium chromium molybdenum tungsten cobalt and gold All the chapters conclude with a summary of the current situation new challenges on the horizon and promising new research directions A list of key reviews and suggestions for further reading also accompanies every chapter Each volume of the Wiley Series on Reactive Intermediates in Chemistry and Biology focuses on a specific reactive intermediate offering a broad range of perspectives from leading experts that sets the stage for new applications and further discoveries

Photoinduced Phenomena in Nucleic Acids I Mario Barbatti, Antonio Carlos Borin, Susanne Ullrich, 2014-12-26 The series Topics in Current Chemistry presents critical reviews of the present and future trends in modern chemical research The scope of coverage is all areas of chemical science including the interfaces with related disciplines such as biology medicine and materials science The goal of each thematic volume is to give the non specialist reader whether in academia or industry a comprehensive insight into an area where new research is emerging which is of interest to a larger scientific audience Each review within the volume critically surveys one aspect of that topic and places it within the context of the volume as a whole The most significant developments of the last 5 to 10 years are presented using selected examples to illustrate the principles discussed The coverage is not intended to be an exhaustive summary of the field or include large quantities of data but should rather be conceptual concentrating on the methodological thinking that will allow the non specialist reader to understand the information presented Contributions also offer an outlook on potential future developments in the field Review articles for the individual volumes are invited by the volume editors Readership research chemists at universities or in industry graduate students

Reviews of Reactive Intermediate Chemistry Matthew S. Platz, Robert A. Moss, Maitland Jones, Jr., 2007-03-22 The chemistry of reactive intermediates is central to a modern mechanistic and quantitative understanding of organic chemistry Moreover it underlies a significant portion of modern synthetic chemistry and is integral to a molecular view of biological chemistry Reviews in Reactive Intermediate Chemistry presents an up to date authoritative guide to this fundamental topic Although it follows Reactive Intermediate Chemistry by the same authors it serves as a free standing resource for the entire chemical and biochemical community The book includes Relevant practical applications Coverage of such topics as mass spectrometry methods reactive intermediates in interstellar medium quantum mechanical tunnelling solvent effects reactive intermediates in biochemical processes and excited state surfaces Discussions of emerging areas particularly those involving dynamics and theories Concluding sections identifying key directions for future research are provided at the end of each chapter

Photophysics and Photochemistry of a BODIPY-Based Photosensitizer Karl Michael Ziems, 2019-04-24 Karl Michael Ziems investigates a meso mesityl 2,6 Iodine substituted Boron Dipyrromethene BODIPY dye regarding its functionality as photosensitizer in a two component light driven hydrogen evolution The author

uses quantum chemical calculations performed at the time dependent density functional TDDFT and multi state restricted active space perturbation theory through second order MS RASPT2 level of theory The light induced processes associated with the formation of the active photosensitizer i e by means of charge separation as well as the population of undesired degradative pathways are elucidated Hereby the two proposed and investigated mechanisms are based on a heavy atom effect of iodine in the excited singlet triplet manifold and preliminary reduction of the dye by a sacrificial electron donor and subsequent photoexcitation

Computational Modelling of Electronic Excited States Eric Bremond, François Maurel, Antonio Monari, 2025-08-01

Computational Modelling of Electronic Excited State provides a comprehensive overview of computational photochemistry and photophysics including both static and dynamic approaches focusing on the challenges and state of the art of the development of original methods for the treatment of electronically excited states both in a density functional theory and wave function framework Despite their widespread presence and their fundamental importance precise characterization at a molecular and electronic level of the underlining mechanisms remains challenging at both an experimental and theoretical level This book provides an exhaustive description of the approaches and methods used to describe with in silico approaches complex photochemical and photophysical processes in complex environments ranging from biology to material science Parts I to III are devoted to methodological development reviewing and explaining the basic principles behind currently used approaches whilst highlighting their strengths and weaknesses to guide early stage researchers in choosing the most suitable approach to take They tackle the key questions What is the validity of method X and in which case can it be used Which method will be most likely available going forwards The book also provides novel critical discussion of emerging approaches gaining traction such as machine learning and quantum computing Parts IV and V of the book then critically present applications involving different domains and different time scales clearly presenting the possibilities offered by molecular modelling and simulation to describe photochemistry and photophysics The questions posed here are Which method is available for the problem Y involving the Z time scale How can I use method X for my specific problem Practical considerations feature throughout involving specific examples to show where some approaches are useful or not suitable and advising on the most profitable use of HPC resources and compatibility Applications belonging to the domain of nanoscience plasmonic and photobiology are presented and critically discussed to show the maturity of the field and the capacity of in silico approaches to answer to key chemical and biological questions

Computational Modelling of Electronic Excited State will be an invaluable resource for computational and experimental oriented researchers working in the field of molecular modelling and simulations with a specific interest in photo induced phenomena as well as graduate students and post doctoral fellows who want to familiarize themselves with the concepts and applications of theoretical photochemistry In addition experimentalists working in the field of time resolved spectroscopy photobiology and photochemistry will benefit from understanding the concepts outlined in the book Gives a comprehensive overview of the

main methods for excited states including dynamic and static approaches including a focus on emerging strategies which have been previously under explained and reviewed Describes a wide range of applications coming from chemistry materials science and biology and spanning different spatial and temporal scales Presents novel topics including attosecond photochemistry and machine learning approaches Provides the reader with the capacity to properly choose the most suitable method for a specific problem via extended review of methodological development applications and perspectives on future directions

Photochemistry Maurizio Persico, Giovanni Granucci, 2018-05-04 This book offers an introduction to photochemistry for students with a minimal background in physical chemistry and molecular quantum mechanics The focus is from a theoretical perspective and highlights excited state dynamics The authors experienced lecturers describe the main concepts in photochemical and photophysical processes that are used as a basis to interpret classical steady state experimental results essentially product branching ratios and quantum yields and the most advanced time resolved techniques A significant portion of the content is devoted to the computational techniques present in quantum chemistry and molecular dynamics With its short summaries questions and exercises this book is aimed at graduate students while its theoretical focus differentiates it from most introductory textbooks on photochemistry

Photochemistry Stefano Protti, Carlotta Raviola, 2020-11-09 This volume combines reviews on the latest advances in photochemical research with specific topical highlights in the field Starting with periodical reports of the recent literature on organic and computational aspects including reports on computational photochemistry and chemiluminescence of biological and nanotechnological molecules photochemistry of alkenes dienes and polyenes aromatic compounds and oxygen containing functions The final chapter of this section is a review of industrial application of photochemistry from 2014 to 2019 Coverage continues with highlighted topics in the second part from ruthenium caged bioactive compounds advances in logically and light induced systems developments of metal free photocatalysts photoresponsive organophosphorus materials and applications of photo fragmentation in synthesis photo click chemistry and azo based molecular photoswitches This volume will again include a section entitled SPR Lectures on Photochemistry a collection of examples for academic readers to introduce a photochemistry topic and precious help for students in photochemistry Providing critical analysis of the topics this book is essential reading for anyone wanting to keep up to date with the literature on photochemistry and its applications A certain amount of energy destroys the same amount of CO₂ according to the whether it is administered continuously or intermittently In order to rationalize this result there are two possibilities either the destruction of CO₂ further occurred in the dark periods which would lead to the same form of energy storing form or in the illuminated period the reaction goes at twice the rate O Warburg Biochem Z 1919 100 230 270

Atomic and Molecular Data and Their Applications Evelyne Roueff, 2007-04-20 This book contains papers presented at the International Conference on Atomic and Molecular Data and their Applications This conference provides a forum for the interaction of Atomic and Molecular AM data producers and users

and for information exchange on AM data needs and availability AM data activities and databases worldwide A
Computational and Experimental Investigation of the Photochemistry of Cyclodecanone Shaei-yun Huang,1991 X-ray
Crystallographic Studies of Cellular Retinoic Acid-binding Protein II Mutants Designed as Rhodopsin Mimics
Xiaofei Jia,2008 **Non-adiabatic Effects in Chemical Dynamics** Royal Society of Chemistry (Great Britain). Faraday
Division,2004 **Computational Photochemistry of Heteroaromatic Biomolecules** L. Therese Bergendahl,2015

Reviews in Computational Chemistry, Volume 15 Kenny B. Lipkowitz,Donald B. Boyd,2009-09-22 THIS VOLUME
WHICH IS DESIGNED FOR STAND ALONE USE IN TEACHING AND RESEARCH FOCUSES ON QUANTUM CHEMISTRY AN
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AND REVIEWS COVER HOW TO OBTAIN SIMPLE CHEMICAL INSIGHT AND CONCEPTS FROM DENSITY FUNCTIONAL
THEORY CALCULATIONS HOW TO MODEL PHOTOCHEMICAL REACTIONS AND EXCITED STATES AND HOW TO
COMPUTE ENTHALPIES OF FORMATION OF MOLECULES A FOURTH CHAPTER TRACES CANADIAN RESEARCH IN THE
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