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Strategies and Applications in Quantum Chemistry

edited by

Y. ELLINGER and M. DEFRANCESCHI

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Strategies And Applications In Quantum Chemistry From Molecular Astrophysics To Molecular Engineering

M Lipman



Strategies And Applications In Quantum Chemistry From Molecular Astrophysics To Molecular Engineering:

Strategies and Applications in Quantum Chemistry Y. Ellinger, M. Defranceschi, 2006-04-11 At the time when increasing numbers of chemists are being attracted by the fascination of supposedly easy computing and associated colourful imaging this book appears as a counterpoint The first part focuses on fundamental concepts of quantum chemistry covering MCSCF theory perturbation treatments basis set developments density matrices wave function instabilities to correlation effects and momentum space theory The second part is devoted to more practical studies ranging from the characterisation of exotic interstellar molecules the accurate determination of spectroscopic constants excited states structures and EPR parameters through photochemical and charge transfer processes cluster chemistry and fullerenes muonium chemistry to the possible prediction of the response of materials to electric fields in view of nonlinear optical applications Audience Graduate students and researchers whose work involves quantum chemistry molecular physics and materials modelling Quantum Systems in Chemistry and Physics. Trends in Methods and Applications R. McWeeny, Jean Maruani, Y.G. Smeyers, S. Wilson, 1998-01-31 Quantum Systems in Chemistry and Physics contains a refereed selection of the papers presented at the first European Workshop on this subject held at San Miniato near Pisa Italy in April 1996 The Workshop brought together leading experts in theoretical chemistry and molecular physics with an interest in the quantum mechanical many body problem This volume provides an insight into the latest research in this increasingly important field Throughout the Workshop the emphasis was on innovative theory and conceptual developments rather than on computational implementation The various contributions presented reflect this emphasis and embrace topics such as density matrices and density functional theory relativistic formulations electron correlation valence theory nuclear motion response theory condensed matter and chemical reactions Audience The volume will be of interest to those working in the molecular sciences and to theoretical chemists and molecular physicists in particular **Strategies and Applications in Quantum Chemistry** Y Ellinger, M Defranceschi, 2014-01-15 At the time when increasing numbers of chemists are being attracted by the fascination of supposedly easy computing and associated colourful imaging this book appears as a counterpoint The first part focuses on fundamental concepts of quantum chemistry covering MCSCF theory perturbation treatments basis set developments density matrices wave function instabilities to correlation effects and momentum space theory The second part is devoted to more practical studies ranging from the characterisation of exotic interstellar molecules the accurate determination of spectroscopic constants excited states structures and EPR parameters through photochemical and charge transfer processes cluster chemistry and fullerenes muonium chemistry to the possible prediction of the response of materials to electric fields in view of nonlinear optical applications Audience Graduate students and researchers whose work involves quantum chemistry molecular physics and materials modelling **Exploring Aspects of Computational Chemistry** Jean-Marie André, 1997 Pris ensemble les deux volumes offrent une introduction théorique et pratique la chimie quantique statistique Ce livre s'adresse un public spécialisé

tudiants de licence doctorants chercheurs *Advances in Computational Methods in Sciences and Engineering 2005 (2 vols)* Theodore Simos, George Maroulis, 2022-05-04 This volume brings together selected contributed papers presented at the International Conference of Computational Methods in Science and Engineering ICCMSE 2005 held in Greece 21 aEURO 26 October 2005 The conference aims to bring together computational scientists from several disciplines in order to share methods and ideas The ICCMSE is unique in its kind It regroups original contributions from all fields of the traditional Sciences Mathematics Physics Chemistry Biology Medicine and all branches of Engineering It would be perhaps more appropriate to define the ICCMSE as a conference on computational science and its applications to science and engineering Topics of general interest are Computational Mathematics Theoretical Physics and Theoretical Chemistry Computational Engineering and Mechanics Computational Biology and Medicine Computational Geosciences and Meteorology Computational Economics and Finance Scientific Computation High Performance Computing Parallel and Distributed Computing Visualization Problem Solving Environments Numerical Algorithms Modelling and Simulation of Complex System Web based Simulation and Computing Grid based Simulation and Computing Fuzzy Logic Hybrid Computational Methods Data Mining Information Retrieval and Virtual Reality Reliable Computing Image Processing Computational Science and Education etc More than 800 extended abstracts have been submitted for consideration for presentation in ICCMSE 2005 From these 500 have been selected after international peer review by at least two independent reviewers *Advances in Molecular Similarity* R. Carbó-Dorca, P.G. Mezey, 1999-02-18 This volume highlights some of the advances in molecular similarity Molecular similarity research is a dynamic field where the rapid transfer of ideas and methodologies from the theoretical quantum chemical and mathematical chemistry disciplines to efficient algorithms and computer programs used in industrially important applications is especially evident These applications often serve as motivating factors toward new advances in the fundamental and theoretical fields and the combination of intellectual challenge and practical utility provides mutual advantages to theoreticians and experimentalists The aim of this volume is to present an overview of the current methodologies of molecular similarity studies and to point out new challenges unsolved problems and areas where important new advances can be expected *Computational and Experimental Chemistry* Tanmoy Chakraborty, Michael J. Bucknum, Eduardo A. Castro, 2013-09-24 This book covers a range of new research on computational quantum chemistry along with a special section devoted to exotic carbon allotropes and spiro quantum theory The section on spiro quantum theory covers the technical presentation of the ideas surrounding the emergence of a synthetic analytical and theoretical spiro quantum chemistry edifi **Chemical Abstracts Service Source Index** American Chemical Society. Chemical Abstracts Service, 1907 A key source to journal and conference abbreviations in the sciences Although it focuses on chemistry other scientific and engineering disciplines are also well represented In addition to the abbreviation and full title each entry also contains publishing info title changes language and frequency of publication and libraries owning that title Over 130 000

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