Computational Chemistry Introduction To The Theory And Applications Of Molecular And Quantum Mechanics

Computational Organic Chemistry
Computational Chemistry
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Mathematical Challenges from Theoretical/Computational Chemistry
Fundamentals, Methods and Applications
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Applications in Industry, Pharma, and Materials Science
An Introduction
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A Concise Introduction
Theoretical and Computational Chemistry
Handbook of Computational Chemistry
Practical Aspects of Computational Chemistry V
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An Introduction to Theoretical Chemistry
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A Practical Guide for Applying Techniques to Real World Problems
Introduction to Theoretical Organic Chemistry and Molecular Modelling
Mathematical Models and Methods for Ab Initio Quantum Chemistry
Computational Quantum Chemistry
An Interactive Introduction to Basis Set Theory
Introduction to Advanced Electronic Structure Theory
A Guide for Materials Scientists, Chemists, Physicists and others
Computational Chemistry
Computational Chemistry
Introduction to Computational Chemistry

Computational Techniques in Quantum Chemistry and Molecular Physics
Introduction to the Theory and Applications of Molecular and Quantum Mechanics
Introduction to the Theory and Applications of Molecular and Quantum Mechanics
Computational Medicinal Chemistry for Drug Discovery
New Horizons in Chemistry

ZANDER COLTON

Computational Organic Chemistry Springer Science & Business Media
Computational Quantum Chemistry removes much of the mystery of modern computer programs for molecular orbital calculations by showing how to develop Excel spreadsheets to perform model calculations and investigate the properties of basis sets. Using the book together with the CD-ROM provides a unique interactive learning tool. In addition, because of the integration of theory with working examples on the CD-ROM, the reader can apply advanced features available in the spreadsheet to other applications in chemistry, physics, and a variety of disciplines that require the solution of differential equations. This book and CD-ROM makes a valuable companion for instructors, course designers, and students. It is suitable for direct applications in practical courses in theoretical chemistry and atomic physics, as well as for teaching advanced features of Excel in IT courses.
Computational Chemistry Springer
This book addresses the construction and application of the major types of basis sets for computational chemistry calculations. In addition to a general introduction, it includes mathematical basics and a discussion of errors arising from incomplete or inappropriate basis sets. The different chapters introduce local orbitals and orbital localization as well as Slater-type orbitals and review basis sets for special applications, such as those for correlated methods, solid-state calculations, heavy atoms and time-dependent adaptable Gaussian bases for quantum dynamics simulations. This detailed review of the purpose of basis sets, their design, applications, possible problems and available solutions provides graduate students and beginning researchers with information not easily obtained from the available textbooks and offers valuable supporting material for any quantum chemistry or computational chemistry course at the graduate and/or undergraduate level. This book is also useful as a guide for researchers who are new to computational chemistry but are willing to extend their research tools by applying such methods.
Computational Chemistry Royal Society of Chemistry
Essentials of Computational Chemistry provides a balanced introduction to this dynamic subject. Suitable for both experimentalists and theorists, a wide range of samples and applications are included drawn from all key areas. The book carefully leads the reader thorough the necessary equations providing information explanations and reasoning where necessary and firmly placing each equation in context.
Mathematical Challenges from Theoretical/Computational Chemistry John Wiley & Sons
Annual Reports in Computational Chemistry is a new periodical providing timely and critical reviews of important topics in computational chemistry as applied to all chemical disciplines. Topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings. Each volume is organized into (thematic) sections with contributions written by experts. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Annual Reports in Computational Chemistry is a 'must' for researchers and students wishing to stay up-to-date on current developments in computational chemistry. * Broad coverage of computational chemistry and up-to-date information * The topics covered include quantum chemistry, molecular mechanics, force fields, chemical education, and applications in academic and industrial settings * Each chapter reviews the most recent literature on a specific topic of interest to computational chemists
Fundamentals, Methods and Applications Springer Nature
The renowned Oxford Chemistry Primers series, which provides focused introductions to a range of important topics in chemistry, has been refreshed and updated to suit the needs of today's students, lecturers, and postgraduate researchers. The rigorous, yet accessible, treatment of each subject area is ideal for those wanting a primer in a given topic to prepare them for more advanced study orresearch.Computational Chemistry provides a user-friendly introduction to this powerful way of characterizing and modelling chemical systems. This primer provides the perfect introduction to the subject, leading the reader through thebasic principles before showing a variety of ways in which computational chemistry is applied in practice to study real molecules, all illustrated by frequent examples.
Reviews in Computational Chemistry Walter de Gruyter GmbH & Co KG
This book explores the applications of computational chemistry ranging from the pharmaceutical industry and molecular structure determination to spectroscopy and astrophysics. The authors detail how calculations can be used to solve a wide range of practical challenges encountered in research and industry.
Applications in Industry, Pharma, and Materials Science National Academies Press
The gap between introductory level textbooks and highly specialized monographs is filled by this modern textbook. It provides in one comprehensive volume the in-depth theoretical background for molecular modeling and detailed descriptions of the applications in chemistry and related fields like drug design, molecular sciences, biomedical, polymer and materials engineering. Special chapters on basic mathematics and the use of respective software tools are included. Numerous numerical examples, exercises and explanatory illustrations as well as a web site with application tools (http://www.amrita.edu/cen/ccmm) support the students and lecturers.
An Introduction Courier Corporation

This is the third edition of the successful text-reference book that covers computational chemistry. It features changes to the presentation of key concepts and includes revised and new material with several expanded exercises at various levels such as 'harder questions' for those ready to be tested in greater depth - this aspect is absent from other textbooks in the field. Although introductory and assuming no prior knowledge of computational chemistry, it covers the essential aspects of the subject. There are several introductory textbooks on computational chemistry; this one is (as in its previous editions) a unique textbook in the field with copious exercises (and questions) and solutions with discussions. Noteworthy is the fact that it is the only book at the introductory level that shows in detail yet clearly how matrices are used in one important aspect of computational chemistry. It also serves as an essential guide for researchers, and as a reference book.

Frontiers in Computational Chemistry Walter de Gruyter GmbH & Co KG

Computational Quantum Chemistry, Second Edition, is an extremely useful tool for teaching and research alike. It stipulates information in an accessible manner for scientific investigators, researchers and entrepreneurs. The book supplies an overview of the field and explains the fundamental underlying principles. It also gives the knowledge of numerous comparisons of different methods. The book consists of a wider range of applications in each chapter. It also provides a number of references which will be useful for academic and industrial researchers. It includes a large number of worked-out examples and unsolved problems for enhancing the computational skill of the users. Features Includes comprehensive coverage of most essential basic concepts Achieves greater clarity with improved planning of topics and is reader-friendly Deals with the mathematical techniques which will help readers to more efficient problem solving Explains a structured approach for mathematical derivations A reference book for academicians and scientific investigators Ram Yatan Prasad, PhD, DSc (India), DSc (hc) Colombo, is a Professor of Chemistry and former Vice Chancellor of S.K.M University, Jharkhand, India. Pranita, PhD, DSc (hc) Sri Lanka, FICS, is an Assistant Professor of Chemistry at Vinoba Bhave University, India.

Basis Sets in Computational Chemistry Courier Corporation

Starting with an overview of the theory behind - and demonstrations of the effect of - electric fields on structure and reactivity, this accessible reference work aims to encourage those new to the field to consider harnessing these effects in their own work.

Effects of Electric Fields on Structure and Reactivity University Science Books

The Reviews in Computational Chemistry series brings together leading authorities in the field to teach the newcomer and update the expert on topics centered on molecular modeling, such as computer-assisted molecular design (CAMD), quantum chemistry, molecular mechanics and dynamics, and quantitative structure-activity relationships (QSAR). This volume, like those prior to it, features chapters by experts in various fields of computational chemistry. Topics in Volume 31 include: Lattice-Boltzmann Modeling of Multicomponent Systems: An Introduction Modeling Mechanochemistry from First Principles Mapping Energy Transport Networks in Proteins The Role of Computations in Catalysis The Construction of Ab Initio Based Potential Energy Surfaces Uncertainty Quantification for Molecular Dynamics

Reviews in Computational Chemistry Courier Corporation

Computational methods are rapidly becoming major tools of theoretical, pharmaceutical, materials, and biological chemists. Accordingly, the mathematical models and numerical analysis that underlie these methods have an increasingly important and direct role to play in the progress of many areas of chemistry. This book explores the research interface between computational chemistry and the mathematical sciences. In language that is aimed at non-specialists, it documents some prominent examples of past successful cross-fertilizations between the fields and explores the mathematical research opportunities in a broad cross-section of chemical research frontiers. It also discusses cultural differences between the two fields and makes recommendations for overcoming those differences and generally promoting this interdisciplinary work.

Modern Quantum Chemistry Courier Corporation

Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields Tight-binding DFT More extensive DFT functionals, excited states and time dependent molecular properties Accelerated Molecular Dynamics methods Tensor decomposition methods Cluster analysis Reduced scaling and reduced prefactor methods Additional information is available at: www.wiley.com/go/jensen/computationalchemistry3

Molecular Structure and Properties in Silico Morgan & Claypool Publishers

Computational chemistry has become extremely important in the last decade, being widely used in academic and industrial research. Yet there have been few books designed to teach the subject to nonspecialists. 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. The following concepts are illustrated and their possibilities and limitations are given: - potential energy surfaces; - simple and extended Hückel methods; - ab initio, AM1 and related semiempirical methods; - density functional theory (DFT). Topics are placed in a historical context, adding interest to them and removing much of their apparently arbitrary aspect. The large number of references, to all significant topics mentioned, should make this book useful not only to undergraduates but also to graduate students and academic and industrial researchers.

Computational Chemistry Springer Nature

Classic undergraduate text explores wave functions for the hydrogen atom, perturbation theory, the Pauli exclusion principle, and the structure of simple and complex molecules. Numerous tables and figures.

Modern Quantum Chemistry Royal Society of Chemistry

Introduction to Computational Chemistry 3rd Edition provides a comprehensive account of the fundamental principles underlying different computational methods. Fully revised and updated throughout to reflect important method developments and improvements since publication of the previous edition, this timely update includes the following significant revisions and new topics: Polarizable force fields Tight-binding DFT More extensive DFT functionals, excited states and time dependent molecular properties Accelerated Molecular Dynamics methods Tensor decomposition

methods Cluster analysis Reduced scaling and reduced prefactor methods Additional information is available at: www.wiley.com/go/jensen/computationalchemistry3

Proceedings of the NATO Advanced Study Institute held at Ramsau, Germany, 4–21 September, 1974 Wiley

This book contains the transcripts of the lectures presented at the NATO Advanced study Institute on "Computational Techniques in Quantum Chemistry and Molecular Physics", held at Ramsau, Germany, 4th - 21st Sept. 1974. Quantum theory was developed in the early decades of this century and was first applied to problems in chemistry and molecular physics as early as 1927. It soon emerged however, that it was impossible to con sider any but the simplest systems in any quantita tive detail because of the complexity of Schrodinger's equation which is the basic equation for chemical and molecular physics applications. This remained the si tuation until the development, after 1950, of elec tronic digital computers. It then became possible to attempt approximate solutions of Schrodinger's equa tion for fairly complicated systems, to yield results which were sufficiently accurate to make comparison with experiment meaningful. Starting in the early nineteen sixties in the United States at a few centres with access to good computers an enormous amount of work went into the development and implementation of schemes for approximate solu tions of Schrodinger's equation, particularly the de velopment of the Hartree-Fock self-consistent-field scheme. But it was soon found that the integrals needed for application of the methods to molecular problems are far from trivial to evaluate and cannot be easily approximated.

A Concise Introduction John Wiley & Sons

This is the first book to present both classical and quantum-chemical approaches to computational methods, incorporating the many new developments in this field from the last few years. Written especially for "non"-theoretical readers in a readily comprehensible and implemental style, it includes numerous practical examples of varying degrees of difficulty. Similarly, the use of mathematical equations is reduced to a minimum, focusing only on those important for experimentalists. Backed by many extensive tables containing detailed data for direct use in the calculations, this is the ideal companion for all those wishing to improve their work in solid state research.

Theoretical and Computational Chemistry Springer Science & Business Media

This handbook is a guide to current methods of computational chemistry, explaining their limitations and advantages and providing examples of their applications. The first part outlines methods, the balance of volumes present numerous important applications.

Handbook of Computational Chemistry Springer Science & Business Media

Observing computational chemistry's proven value to the introduction of new medicines, this reference offers the techniques most frequently utilized by industry and academia for ligand design. Featuring contributions from more than fifty pre-eminent scientists, Computational Medicinal Chemistry for Drug Discovery surveys molecular structure computa