Linear Scaling Techniques In Computational Chemistry And Physics Methods And Applications Challenges And Advances In Computational Chemistry And Physics

Fragmentation: Toward Accurate Calculations on Complex Molecular Systems introduces the reader to the broad array of fragmentation and embedding methods that are currently available or under development to facilitate accurate calculations on large, complex systems such as proteins, polymers, liquids and nanoparticles. These methods work by subdividing a system into subunits, called fragments or subsystems or domains. Calculations are performed on each fragment and then the results are combined to predict properties for the whole system. Topics covered include: Fragmentation methods Embedding methods Explicitly correlated local electron correlation methods Fragment molecular orbital method Methods for treating large molecules This book is aimed at academic researchers who are interested in computational chemistry, computational biology, computational materials science and related fields, as well as graduate students in these fields.

Annual Reports in Computational Chemistry provides 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. Focusing on the most recent literature and advances in the field, each article covers a specific topic of importance to computational chemists. Quantum chemistry Molecular mechanics Force fields Chemical education and applications in academic and industrial settings

Most textbooks in the field are either too advanced for students or don't adequately cover current research topics. Bridging this gap, Electronic Structure of Materials helps advanced undergraduate and graduate students understand electronic structure methods and enables them to use these techniques in their work.Developed from the author's lecture

This book provides a comprehensive overview of modern computer-based techniques for analyzing the structure, properties and dynamics of biomolecules and biomolecular processes. It is organized in four main parts; the first one deals with methodology of molecular simulations; the second one with applications of molecular simulations; the third one introduces bioinformatics methods and the use of experimental information in molecular simulations; the last part reports on selected applications of molecular quantum mechanics. This second edition has been thoroughly revised and updated to include the latest progresses made in the respective field of research.

In-depth overview of two-dimensional semiconductors from theoretical studies, properties to emerging applications! Two-dimensional (2D) materials have attracted enormous attention due to their exotic properties deriving from their ultrathin dimensions. 2D materials, such as graphene, transition metal dichalcogenides, transition metal oxides, black phosphorus and boron nitride, exhibit versatile optical, electronic, catalytic and mechanical properties, thus can be used in a wide range of applications, including electronics, optoelectronics and optical applications. Two-Dimensional Semiconductors: Synthesis, Physical Properties and Applications provides an in-depth view of 2D semiconductors from theoretical studies, properties to applications, taking into account the current state of research and development. It introduces various preparation methods and describes in detail the physical properties of 2D semiconductors including 2D alloys and heterostructures. The covered applications include, but are not limited to, field-effect transistors, spintronics, solar cells, photodetectors, light-emitting diode, sensors and bioelectronics. * Highly topical: 2D materials are a rapidly advancing field that attracts increasing attention * Concise overview: covers theoretical studies, preparation methods, physical properties, potential applications, the challenges and opportunities * Application oriented: focuses on 2D semiconductors that can be used in various applications such as field-effect transistors, solar cells, sensors and bioelectronics * Highly relevant: newcomers as well as experienced researchers in the field of 2D materials will benefit from this book Two-Dimensional Semiconductors: Synthesis, Physical Properties and Applications is written for materials scientists, semiconductor and solid state physicists, electrical engineers, and readers working in the semiconductor industry.

While its results normally complement the information obtained by chemical experiments, computer computations can in some cases predict unobserved chemical phenomena Electronic-Structure Computational Methods for Large Systems gives readers a simple description of modern electronic-structure techniques. It shows what techniques are pertinent for particular problems in biotechnology and nanotechnology and provides a balanced treatment of topics that teach strengths and weaknesses, appropriate and inappropriate methods. It’s a book that will enhance the your calculating confidence and improve your ability to predict new effects and solve new problems.

A practical, easily accessible guide for bench-top chemists, thisbook focuses on accurately applying computational chemistrytechniques to everyday chemistry problems. Provides nonmathematical explanations of advanced topics incomputational chemistry. Focuses on when and how to apply different computationaltechniques. Addresses computational chemistry connections to biochemicalsystems and polymers. Provides a prioritized list of methods for attacking difficultcomputational chemistry problems, and compares advantages anddisadvantages of various approximation techniques. Describes how the choice of methods of software affectsrequirements for computer memory and processing time.

The methodological development and computational implementation of linear scaling quantum chemistry methods for the accurate calculation of electronic structure and properties of periodic systems (solids, surfaces, and polymers) and their application to chemical problems of DOE relevance.

Issues in Computation / 2013 Edition is a ScholarlyEditions™ book that delivers timely, authoritative, and comprehensive information about Computing. The editors have built Issues in Computation: 2013 Edition on the vast information databases of ScholarlyNews.™ You can expect the information about Computing in this book to be deeper than what you can access anywhere else, as well as consistently reliable, authoritative, informed, and relevant. The content of Issues in Computation / 2013 Edition has been produced by the world’s leading scientists, engineers, analysts, research institutions, and companies. All of the content is from peer-reviewed sources, and all of it is written, assembled, and edited by the editors at ScholarlyEditions™ and available exclusively from us. You now have a source you can cite with authority, confidence, and credibility. More information is available at http://www.ScholarlyEditions.com/.

Computational chemistry is a means of applying theoretical ideas using computers and a set of techniques for investigating chemical problems within which common questions vary from molecular geometry to the physical properties of substances. Theory and Applications of Computational Chemistry: The First Forty Years is a collection of articles on the emergence of computational chemistry. It shows the enormous breadth of theoretical and computational chemistry today and establishes how theory and computation have become increasingly linked as methodologies and technologies have advanced. Written by the pioneers in the field, the book presents historical perspectives and insights into the subject, and addresses new and current methods, as well as problems and applications in theoretical and computational chemistry. Easy to read and packed with personal insights, technical and classical information, this book provides the perfect introduction for graduate students beginning research in this area. It also provides very readable and useful reviews for theoretical chemists. * Written by well-known leading experts * Combines history, personal accounts, and theory to explain much of the field of theoretical and compuational chemistry * Is the perfect introduction to the field

Trends in Computational Nanomechanics reviews recent advances in analytical and computational modeling frameworks to describe the mechanics of materials on scales ranging from the atomistic, through the microstructure or transitional, and up to the continuum. The book presents new approaches in the theory of nanosystems, recent developments in theoretical and computational methods for studying problems in which multiple length and/or time scales must be simultaneously resolved, as well as example applications in nanomechanics. This title will be a useful tool of reference for professionals, graduates and undergraduates interested in Computational Chemistry and Physics, Materials Science, Nanotechnology.

A systematic discussion of the fundamental principles, written by a leading contributor to the field.

Ab initio quantum chemistry has emerged as an important tool in chemical research and is appliced to a wide variety of problems in chemistry and molecular physics. Recent developments of computational methods have enabled previously intractable chemical problems to be solved using rigorous quantum-mechanical methods. This is the first comprehensive, up-to-date and technical work to cover all the important aspects of modern molecular electronic-structure theory. Topics covered in the book include: * Second quantization with spin adaptation * Gaussian basis sets and molecular-integral evaluation * Hartree-Fock theory * Configuration-interaction and multi-configurational self-consistent theory * Coupled-cluster theory for ground and excited states * Perturbation theory for single- and multi-configurational states * Linear-scaling techniques and the fast multipole method * Explicity correlated wave functions * Basis-set convergence and extrapolation * Calibration and benchmarking of computational methods, with applications to moelcular equilibrium structure, atomization energies and reaction enthalpies. Molecular Electronic-Structure Theory makes extensive use of numerical examples, designed to illustrate the strengths and weaknesses of each method treated. In addition, statements about the usefulness and deficiencies of the various methods are supported by actual examples, not just model calculations. Problems and exercises are provided at the end of each chapter, complete with hints and solutions. This book is a must for researchers in the field of quantum chemistry as well as for nonspecialists who wish to acquire a thorough understanding of ab initio molecular electronic-structure theory and its applications to problems in chemistry and physics. It is also highly recommended for the teaching of graduates and advanced undergraduates.

In this Festschrift dedicated to the 60th birthday of Péter R. Surján, selected researchers in theoretical chemistry present research highlights on major developments in the field. Originally published in the journal Theoretical Chemistry Accounts, these outstanding contributions are now available in a hardcover print format, as well as a special electronic edition. This volume provides valuable content for all researchers in theoretical chemistry and will especially benefit those research groups and libraries with limited access to the journal.

Computational Quantum Chemistry presents computational electronic structure theory as practised in terms of ab initio waveform methods and density functional approaches. Getting a full grasp of the field can often prove difficult, since essential topics fall outside of the scope of conventional chemistry education. This professional reference book provides a comprehensive introduction to the field. Postgraduate students and experienced researchers alike will appreciate Joseph McDouall's engaging writing style. The book is divided into five chapters, each providing a major aspect of the field. Electronic structure methods, the computation of molecular properties, methods for analysing the output from computations and the importance of relativistic effects on molecular properties are also discussed. Links to the websites of widely used software packages are provided so that the reader can gain first hand experience of using the techniques described in the book. Dr McDouall has more than 25 years experience in theoretical chemistry; as a reader at the University of Manchester his research interests include the application of quantum chemical methods to the elucidation of chemical problems and the development and implementation of electronic structure methods that permit the accurate prediction of chemical structures and molecular properties.

Proceedings of the International Symposium on Supercomputing held in Tokyo, Japan, September 1-3, 1997

Illustrates the application of mathematical and computational modeling in a variety of disciplines With an emphasis on the interdisciplinary nature of mathematical and computational modeling, Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts features chapters written by well-known, international experts in these fields and presents readers with a host of state-of-the-art achievements in the development of mathematical modeling and computational experiment methodology. The book is a valuable guide to the methods, ideas, and tools of applied and computational mathematics as they apply to other disciplines such as the natural and social sciences, engineering, and technology. Mathematical and Computational Modeling: With Applications in the Natural and Social

Sciences, Engineering, and the Arts also features: Rigorous mathematical procedures and applications as the driving force behind mathematical innovation and discovery Numerous examples from a wide range of disciplines to emphasize the multidisciplinary application and universality of applied mathematics and mathematical modeling Original results on both fundamental theoretical and applied developments in diverse areas of human knowledge Discussions that promote interdisciplinary interactions between mathematicians, scientists, and engineers Mathematical and Computational Modeling: With Applications in the Natural and Social Sciences, Engineering, and the Arts is an ideal resource for professionals in various areas of mathematical and statistical sciences, modeling and simulation, physics, computer science, engineering, biology and chemistry, industrial, and computational engineering. The book also serves as an excellent textbook for graduate courses in mathematical modeling, applied mathematics, numerical methods, operations research, and optimization.

London dispersion interactions are responsible for numerous phenomena in physics, chemistry and biology. Recent years have seen the development of new, physically well-founded models, and dispersion-corrected density functional theory (DFT) is now a hot topic of research. This book is an overview of current understanding of the physical origin and modelling of London dispersion forces manifested at an atomic level. It covers a wide range of system, from small intermolecular complexes, to organic molecules and crystalline solids, through to biological macromolecules and nanostructures. In presenting a broad overview of the of the physical foundations of dispersion forces, the book provides theoretical, physical and synthetic chemists, as well as solid-state physicists, with a systematic understanding of the origins and consequences of these ubiquitous interactions. The presentation is designed to be accessible to anyone with intermediate undergraduate mathematics, physics and chemistry.

From the Foreword: "The authors of the chapters in this book are the pioneers who will explore the exascale frontier. The path forward will not be easy... These authors, along with their colleagues who will produce these powerful computer systems will, with dedication and determination, overcome the scalability problem, discover the new algorithms needed to achieve exascale performance for the broad range of applications that they represent, and create the new tools needed to support the development of scalable and portable science and engineering applications. Although the focus is on exascale computers, the benefits will permeate all of science and engineering because the technologies developed for the exascale computers of tomorrow will also power the petascale servers and terascale workstations of tomorrow. These affordable computing capabilities will empower scientists and engineers everywhere." — Thom H. Dunning, Jr., Pacific Northwest National Laboratory and University of Washington, Seattle, Washington, USA "This comprehensive summary of applications targeting Exascale at the three DoE labs is a must read." — Rio Yokota, Tokyo Institute of Technology, Tokyo, Japan "Numerical simulation is now a need in many fields of science, technology, and industry. The complexity of the simulated systems coupled with the massive use of data makes HPC essential to move towards predictive simulations. Advances in computer architecture have so far permitted scientific advances, but at the cost of continually adapting algorithms and applications. The next technological breakthroughs force us to rethink the applications by taking energy consumption into account. These profound modifications require not only anticipation and sharing but also a paradigm shift in application design to ensure the sustainability of developments by guaranteeing a certain independence of the applications to the profound modifications of the architectures: it is the passage from optimal performance to the portability of performance. It is the challenge of this book to demonstrate by example the approach that one can adopt for the development of applications offering performance portability in spite of the profound changes of the computing architectures." — Christophe Calvin, CEA, Fundamental Research Division, Saclay, France "Three editors, one from each of the High Performance Computer Centers at Lawrence Berkeley, Argonne, and Oak Ridge National Laboratories, have compiled a very useful set of chapters aimed at describing software developments for the next generation exa-scale computers. Such a book is needed for scientists and engineers to see where the field is going and how they will be able to exploit such architectures for their own work. The book will also benefit students as it provides insights into how to develop software for such computer architectures. Overall, this book fills an important need in showing how to design and implement algorithms for exa-scale architectures which are heterogeneous and have unique memory systems. The book discusses issues with developing user codes for these architectures and how to address these issues including actual coding examples.' — Dr. David A. Dixon, Robert Ramsay Chair, The University of Alabama, Tuscaloosa, Alabama, USA

This work addresses the computation of excited-state properties of systems containing thousands of atoms. To achieve this, the author combines the linear response formulation of time-dependent density functional theory (TDDFT) with linear-scaling techniques known from ground-state density-functional theory. This extends the range of TDDFT, which on its own cannot tackle many of the large and interesting systems in materials science and computational biology. The strengths of the approach developed in this work are demonstrated on a number of problems involving large-scale systems, including exciton coupling in the Fenna-Matthews-Olson complex and the investigation of low-lying excitations in doped p-terphenyl organic crystals.

THIS VOLUME, LIKE THOSE PRIOR TO IT, FEATURES CHAPTERS BY EXPERTS IN VARIOUS FIELDS OF COMPUTATIONAL CHEMISTRY. Volume 23 COVERS LINEAR SCALING METHODS FOR QUANTUM CHEMISTRY, VARIATIONAL TRANSITION STATE THEORY, COARSE GRAIN MODELING OF POLYMERS, SUPPORT VECTOR MACHINES, CONICAL INTERSECTIONS, ANALYSIS OF INFORMATION CONTENT USING SHANNON ENTROPY, AND HISTORICAL INSIGHTS INTO HOW COMPUTING EVOLVED IN THE PHARMACEUTICAL INDUSTRY. FROM REVIEWS OF THE SERIES "Reviews in Computational Chemistry remains the most valuable reference to methods and techniques in computational chemistry." —JOURNAL OF MOLECULAR GRAPHICS AND MODELLING "One cannot generally do better than to try to find an appropriate

article in the highly successful Reviews in Computational Chemistry. The basic philosophy of the editors seems to be to help the authors produce chapters that are complete, accurate, clear, and accessible to experimentalists (in particular) and other nonspecialists (in general)." —JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

This book presents theoretical studies of electronic structure, optical and spectroscopic properties of a number of compounds such as porphyrins, fullerenes and heteroatomic single-wall nanotubes. The book presents new, faster calculation methods for application in quantum-chemical theory of electronic structures. It addresses issues of practical importance such as the development of materials for photosensitizers, organic LEDs and solar cells.

This book treats state-of-the-art computational methods for power flow studies and contingency analysis. In the first part the authors present the relevant computational methods and mathematical concepts. In the second part, power flow and contingency analysis are treated. Furthermore, traditional methods to solve such problems are compared to modern solvers, developed using the knowledge of the first part of the book. Finally, these solvers are analyzed both theoretically and experimentally, clearly showing the benefits of the modern approach.

This quite simply superb book focuses on various techniques of computational intelligence, both single ones and those which form hybrid methods. These techniques are today commonly applied to issues of artificial intelligence. The book presents methods of knowledge representation using different techniques, namely the rough sets, type-1 fuzzy sets and type-2 fuzzy sets. Next up, various neural network architectures are presented and their learning algorithms are derived. Then, the family of evolutionary algorithms is discussed, including connections between these techniques and neural networks and fuzzy systems. Finally, various methods of data partitioning and algorithms of automatic data clustering are given and new neuro-fuzzy architectures are studied and compared.

Computational and Data-Driven Chemistry Using Artificial Intelligence: Volume 1: Fundamentals, Methods and Applications highlights fundamental knowledge and current developments in the field, giving readers insight into how these tools can be harnessed to enhance their own work. Offering the ability to process large or complex data-sets, compare molecular characteristics and behaviors, and help researchers design or identify new structures, Artificial Intelligence (AI) holds huge potential to revolutionize the future of chemistry. Volume 1 explores the fundamental knowledge and current methods being used to apply AI across a whole host of chemistry applications. Drawing on the knowledge of its expert team of global contributors, the book offers fascinating insight into this rapidly developing field and serves as a great resource for all those interested in exploring the opportunities afforded by the intersection of chemistry and AI in their own work. Part 1 provides foundational information on AI in chemistry, with an introduction to the field and guidance on database usage and statistical analysis to help support newcomers to the field. Part 2 then goes on to discuss approaches currently used to address problems in broad areas such as computational and theoretical chemistry; materials, synthetic and medicinal chemistry; crystallography, analytical chemistry, and spectroscopy. Finally, potential future trends in the field are discussed. Provides an accessible introduction to the current state and future possibilities for AI in chemistry Explores how computational chemistry methods and approaches can both enhance and be enhanced by AI Highlights the interdisciplinary and broad applicability of AI tools across a wide range of chemistry fields

"Linear-Scaling Techniques in Computational Chemistry and Physics" summarizes recent progresses in linear-scaling techniques and their applications in chemistry and physics. In order to meet the needs of a broad community of chemists and physicists, the book focuses on recent advances that extended the scope of possible exploitations of the theory. The first chapter provides an overview of the present state of the linear-scaling methodologies and their applications, outlining hot topics in this field, and pointing to expected developments in the near future. This general introduction is then followed by several review chapters written by experts who substantially contributed to recent developments in this field. The purpose of this book is to review, in a systematic manner, recent developments in linear-scaling methods and their applications in computational chemistry and physics. Great emphasis is put on the theoretical aspects of linear-scaling methods. This book serves as a handbook for theoreticians, who are involved in the development of new efficient computational methods as well as for scientists, who are using the tools of computational chemistry and physics in their research.

This special volume collects invited articles by participants of the Third International Workshop on Methods for Macromolecular Modeling, Courant Institute of Mathematical Sciences, Oct. 12-14, 2000. Leading developers of methods for biomolecular simulations review advances in Monte Carlo and molecular dynamics methods, free energy computational methods, fast electrostatics (particle-mesh Ewald and fast multipole methods), mathematics, and molecular neurobiology, nucleic acid simulations, enzyme reactions, and other essential applications in biomolecular simulations. A Perspectives article by the editors assesses the directions and impact of macromolecular modeling research, including genomics and proteomics. These reviews and original papers by applied mathematicians, theoretical chemists, biomedical researchers, and physicists are of interest to interdisciplinary research students, developers and users of biomolecular methods in academia and industry.

This practical guide describes the basic computational methodologies for catalysis and materials science at an introductory level, presenting the methods with relevant applications, such as spectroscopic properties, chemical reactivity and transport properties of catalytically interesting materials. Edited and authored by internationally recognized scientists, the text provides examples that may be considered and followed as state-of-the art.

Linear-Scaling Techniques in Computational Chemistry and PhysicsMethods and ApplicationsSpringer Science & Business Media

This book offers a theoretical and computational presentation of a variety of linear programming algorithms and methods with an emphasis on the revised simplex method and its components.

A theoretical background and mathematical formulation is included for each algorithm as well as comprehensive numerical examples and corresponding MATLAB® code. The MATLAB® implementations presented in this book are sophisticated and allow users to find solutions to large-scale benchmark linear programs. Each algorithm is followed by a computational study on benchmark problems that analyze the computational behavior of the presented algorithms. As a solid companion to existing algorithmic-specific literature, this book will be useful to researchers, scientists, mathematical programmers, and students with a basic knowledge of linear algebra and calculus. The clear presentation enables the reader to understand and utilize all components of simplex-type methods, such as presolve techniques, scaling techniques, pivoting rules, basis update methods, and sensitivity analysis.

The behaviour of many complex materials extends over time- and lengthscales well beyond those that can normally be described using standard molecular dynamics or Monte Carlo simulation techniques. As progress is coming more through refined simulation methods than from increased computer power, this volume is intended as both an introduction and a review of all relevant modern methods that will shape molecular simulation in the forthcoming decade. Written as a set of tutorial reviews, the book will be of use to specialists and nonspecialists alike.

The theoretical methods of quantum chemistry have matured to the point that accurate predictions can be made and experiments can be understood for a wide range of important gas-phase phenomena. A large part of this success can be attributed to the maturation of hierarchies of approximation, which allow one to approach very high accuracy, provided that sufficient computational resources are available. Until recently, these hierarchies have not been available in condensed-phase chemistry, but recent advances in the field have now led to a group of methods that are capable of reaching this goal. Accurate Condensed-Phase Quantum Chemistry addresses these new methods and the problems to which they can be applied. The book begins with an overview of periodic treatments of electron correlation, with an emphasis on the algorithmic features responsible for their computational efficiency. The first section of the book: Describes the Laplace-transform approach to periodic second-order perturbation theory (MP2) Examines local and density fitted schemes for MP2 in crystalline systems Presents test calculations for a variety of systems with small and medium-sized unit cells The next section focuses on methods based on treatment of the periodic solid in terms of fragments. This part of the book: Explores the incremental many-body scheme for electron correlation in solids, and describes progress towards metals and molecules on surfaces Describes the hierarchical method as an alternative fragment-based approach to electron correlation in crystalline solids, using conventional molecular electronic structure methods Examines electrostatically embedded many-body expansion for large systems, with an emphasis on molecular clusters and molecular liquids Explores delocalized and localized orbital approaches to the electronic structures of periodic and non-periodic solids Lastly, the book describes a practical method by which conventional molecular electronic structure theory can be applied to molecular liquids and solids. Along with the methodology, it presents results on small to medium water clusters as well as on liquid water.

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

An overview of the techniques used to examine supramolecular aggregates from a methodological point of view. Edited by a rising star in the community and an experienced author, this is a definitive survey of useful modern analytical methods for understanding supramolecular chemistry, from NMR to single-molecule spectroscopy, from electron microscopy to extraction methods. A definitive study of this field touching many interdisciplinary areas such as molecular devices, biology, bioorganic chemistry, material science, and nanotechnology.

Nickel Base Single Crystals Across Length Scales is addresses the most advanced knowledge in metallurgy and computational mechanics and how they are applied to superalloys used as bare materials or with a thermal barrier coating system. Joining both aspects, the book helps readers understand the mechanisms driving properties and their evolution from fundamental to application level. These guidelines are helpful for students and researchers who wish to understand issues and solutions, optimize materials, and model them in a cross-check analysis, from the atomistic to component scale. The book is useful for students and engineers as it explores processing, characterization and design. Provides an up-to-date overview on the field of superalloys Covers the relationship between microstructural evolution and mechanical behavior at high temperatures Discusses both basic and advanced modeling and characterization techniques Includes case studies that illustrate the application of techniques presented in the book