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New Directions in Antimatter Chemistry and Physics - Clifford M. Surko 2001-08-31
This book presents a state-of-the-art view of antimatter-matter chemistry and physics, with emphasis on the nanoscopic interactions of positronium atoms with ordinary matter. Selected applications are also discussed. The chapters present a summary of current knowledge in terms of both theory and experiment and as look to the future of research in this area. Extensive bibliographies are included to make the volume a useful reference book. This volume is intended for a broad audience, ranging from specialists in postron research to the graduate students who could use one or a few of the chapters as the introduction to a research area.

Second Quantized Approach to Quantum Chemistry - Peter R. Surjan 2012-12-06
The aim of this book is to give a simple, short, and elementary introduction to the second quantized formalism as applied to a many-electron system. It is intended for those, mainly chemists, who are familiar with traditional quantum chemistry but have not yet become acquainted with second quantization. The treatment is, in part, based on a series of seminars held by the author on the subject. It has been realized that many quantum chemists either interested in theory or in applications, being educated as chemi~ts and not as physicists, have never devoted themselves to taking a course on the second quantized approach. Most available textbooks on this topic are not very easy to follow for those who are not trained in theory, or they are not detailed enough to offer a comprehensive treatment. At the same time there are several papers in quantum chemical literature which take advantage of using second quantization, and it would be worthwhile if those papers were accessible for a wider reading public. For this reason, it is intended in this survey to review the basic formalism of second quantization, and to treat some selected chapters of quantum chemistry in this language. Most derivations will be carried out in a detailed manner, so the reader need not accept gaps to understand the result.

New Electron Correlation Methods and Their Applications, and Use of Atomic Orbitals with Exponential Asymptotes - Monika Musial 2021-09-28
Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry, and biology. It features detailed reviews written by leading international researchers. In this volume the readers are presented with an exciting combination of themes. Presents surveys of current topics in this rapidly-

developing field that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry and biology Features detailed reviews written by leading international researchers

Relativistic Quantum Chemistry - Markus Reiher 2009-05-13

Written by two researchers in the field, this book is a reference to explain the principles and fundamentals in a self-contained, complete and consistent way. Much attention is paid to the didactical value, with the chapters interconnected and based on each other. From the contents: * Fundamentals * Relativistic Theory of a Free Electron: Diraci¿1⁄2s Equation * Dirac Theory of a Single Electron in a Central Potential * Many-Electron Theory I: Quantum Electrodynamics * Many-Electron Theory II: Dirac-Hartree-Fock Theory * Elimination of the Small Component * Unitary Transformation Schemes * Relativistic Density Functional Theory * Physical Observables and Molecular Properties * Interpretive Approach to Relativistic Quantum Chemistry From beginning to end, the authors deduce all the concepts and rules, such that readers are able to understand the fundamentals and principles behind the theory. Essential reading for theoretical chemists and physicists.

Electronic Density Functional Theory - John F. Dobson 1998-04-30

Proceedings of an International Workshop held in Nathan, Australia, July 14-19, 1996

Physics, Chemistry and Application of Nanostructures - V E Borisenko 2005-04-28

This comprehensive volume presents invited reviews and short notes with exciting new results obtained in fabrication study and application of nanostructures, which promise a new generation of electronic and optoelectronic devices. The rapid progress in nanoelectronics and optoelectronics, molecular electronics and spintronics, nanotechnology and quantum processing of information are covered. Contents:Physics of NanostructuresSpintronicsChemistry of NanostructuresNanotechnologyNanostructure Based Devices Readership: Graduate students and researchers in nanoscience and nanotechnology. Keywords:Nanostructures;Nanotechnology;Quantum Computing;Bioinformatics;Nanoelectronics;Spintronics;NanophotonicsKey Features:Provides the most recent collection of results in the fieldCovers areas not presented in any other competing titleContributors are well-known specialists in the field

Quantum Chemistry - David B. Cook 2008

This book is a presentation of a qualitative theory of chemical bonding stressing the physical processes which occur on bond formation. It differs from most (if not all) other books in that it does not seek to ?rationalize? the phenomena of bonding by a series of mnemonic rules. A principal feature is a unified and consistent treatment across all types of bonding in organic, physical and inorganic chemistry.

Quantum Monte Carlo Methods in Physics and Chemistry - M.P. Nightingale 1998-12-31

This book contains lectures on the basic theory and applications of quantum Monte Carlo methods, with contributions written by authorities in the field. Although tutorial in nature, it includes current developments. Both continuum systems and lattice models are covered. The applications include atomic, molecular, and solid state physics, statistical and low-temperature physics, and nuclear structure. Suitable for Ph.D. students and beyond.

Many-Electron Approaches in Physics, Chemistry and Mathematics - Volker Bach 2014-07-01

This book provides a broad description of the development and (computational) application of many-electron approaches from a multidisciplinary perspective. In the context of studying many-electron systems Computer Science, Chemistry, Mathematics and Physics are all intimately interconnected. However, beyond a handful of communities working at the interface between these disciplines, there is still a marked separation of subjects. This book seeks to offer a common platform for possible exchanges between the various fields and to introduce the reader to perspectives for potential further developments across the disciplines. The rapid advances of modern technology will inevitably require substantial improvements in the approaches currently used, which will in turn make exchanges between disciplines indispensable. In

essence this book is one of the very first attempts at an interdisciplinary approach to the many-electron problem.

Quantum Monte Carlo Methods in Physics and Chemistry - M.P. Nightingale 1998-12-31

In recent years there has been a considerable growth in interest in Monte Carlo methods, and quantum Monte Carlo methods in particlular. Clearly, the ever-increasing computational power available to researchers, has stimulated the development of improved algorithms, and almost all fields in computational physics and chemistry are affected by their applications. Here we just mention some fields that are covered in the lecture notes contained in this volume, viz. electronic structure studies of atoms, molecules and solids, nuclear structure, and low- or zero-temperature studies of strongly-correlated quantum systems, both of the continuum and lattice variety, and cooperative phenomena in classical systems. Although each area of application may have its own peculiarities, requiring specialized solutions, all share the same basic methodology. It was with the intention of bringing together researchers and students from these various areas that the NATO Advanced Study Institute on Quantum Monte Carlo Methods in Physics and Chemistry was held at Cornell University from 12 to 24 July, 1998. This book contains material presented at the Institute in a series of mini courses in quantum Monte Carlo methods. The program consisted of lectures predominantly of a pedagogical nature, and of more specialized seminars. The levels varied from introductory to advanced, and from basic methods to applications; the program was intended for an audience working towards the Ph.D. level and above. Despite the essentially pedagogic nature of the Institute, several of the lectures and seminars contained in this volume present recent developments not previously published.

Computational Methods for Electron—Molecule Collisions - Franco A. Gianturco 2013-06-29

The collision of electrons with molecules and molecular ions is a fundamental pro cess in atomic and molecular physics and in chemistry. At high incident electron en ergies, electron-molecule collisions are used to deduce molecular geometries, oscillator strengths for optically allowed transitions, and in the case of electron-impact ionization, to probe the momentum distribution of the molecule itself. When the incident electron energy is comparable to or below those of the molecular valence electrons, the physics involved is particularly rich. Correlation and exchange effects necessary to describe such collision processes bear a close resemblance to similar efft:cts in the theory of electronic structure in molecules. Compound state formations, in the form of resonances and vir tual states, manifest themselves in experimental observables which provide details of the electron-molecule interactions. Ro-vibrational excitations by low-energy electron collisions exemplify energy transfer between the electronic and nuclear motion. The role of nonadiabatic interaction is raised here. When the final vibrational state is in the continuum, molecular dissociation occurs. Dissociative recombination and dissociative attachment are examples of such fragmentation processes. In addition to its fundamental nature, the study of electron-molecule collisions is also motivated by its relation to other fields of study and by its technological appli cations. The study of planetary atmospheres and the interstellar medium necessarily involve collision processes of electrons with molecules and molecular ions.

Energy Density Functional Theory of Many-Electron Systems - Eugene S. Kryachko 2012-12-06

Intermolecular Interactions - Ilya G. Kaplan 2006-05-01

The subject of this book — intermolecular interactions — is as important in physics as in chemistry and molecular biology. Intermolecular interactions are responsible for the existence of liquids and solids in nature. They determine the physical and chemical properties of gases, liquids, and crystals, the stability of chemical complexes and biological compounds. In the first two chapters of this book, the detailed qualitative description of different types of intermolecular forces at large, intermediate and short-range distances is presented. For the first time in the monographic literature, the temperature dependence of the dispersion forces is discussed, and it is shown that at finite temperatures

the famous Casimir-Polder asymptotic formula is correct only at narrow distance range. The author has aimed to make the presentation understandable to a broad scope of readers without oversimplification. In Chapter 3, the methods of quantitative calculation of the intermolecular interactions are discussed and modern achievements are presented. This chapter should be helpful for scientists performing computer calculations of many-electron systems. The last two chapters are devoted to the many-body effects and model potentials. More than 50 model potentials exploited for processing experimental data and computer simulation in different fields of physics, chemistry and molecular biology are represented. The widely used global optimisation methods: simulated annealing, diffusion equation method, basin-hopping algorithm, and genetic algorithm are described in detail. Significant efforts have been made to present the book in a self-sufficient way for readers. All the necessary mathematical apparatus, including vector and tensor calculus and the elements of the group theory, as well as the main methods used for quantal calculation of many-electron systems are presented in the appendices.

Theoretical Chemistry and Physics of Heavy and Superheavy Elements - U. Kaldor 2013-06-29

Quantum mechanics provides the fundamental theoretical apparatus for describing the structure and properties of atoms and molecules in terms of the behaviour of their fundamental components, electrons and nudeL For heavy atoms and molecules containing them, the electrons can move at speeds which represent a substantial fraction of the speed of light, and thus relativity must be taken into account. Relativistic quantum mechanics therefore provides the basic formalism for calculating the properties of heavy-atom systems. The purpose of this book is to provide a detailed description of the application of relativistic quantum mechanics to the many-body prob lem in the theoretical chemistry and physics of heavy and superheavy elements. Recent years have witnessed a continued and growing interest in relativistic quantum chemical methods and the associated computa tional algorithms which facilitate their application. This interest is fu elled by the need to develop robust, yet efficient theoretical approaches, together with efficient algorithms, which can be applied to atoms in the lower part of the Periodic Table and, more particularly, molecules and molecular entities containing such atoms. Such relativistic theories and computational algorithms are an essential ingredient for the description of heavy element chemistry, becoming even more important in the case of superheavy elements. They are destined to become an indispensable tool in the quantum chemist's armoury. Indeed, since relativity influences the structure of every atom in the Periodic Table, relativistic molecular structure methods may replace in many applications the non-relativistic techniques widely used in contemporary research.

Many-Body Methods for Atoms, Molecules and Clusters - Jochen Schirmer 2018-11-02

This book provides an introduction to many-body methods for applications in quantum chemistry. These methods, originating in field-theory, offer an alternative to conventional quantum-chemical approaches to the treatment of the many-electron problem in molecules. Starting with a general introduction to the atomic and molecular many-electron problem, the book then develops a stringent formalism of field-theoretical many-body theory, culminating in the diagrammatic perturbation expansions of many-body Green's functions or propagators in terms of Feynman diagrams. It also introduces and analyzes practical computational methods, such as the field-tested algebraic-diagrammatic construction (ADC) schemes. The ADC concept can also be established via a wave-function based procedure, referred to as intermediate state representation (ISR), which bridges the gap between propagator and wave-function formulations. Based on the current rapid increase in computer power and the development of efficient computational methods, quantum chemistry has emerged as a potent theoretical tool for treating ever-larger molecules and problems of chemical and physical interest. Offering an introduction to many-body methods, this book appeals to advanced students interested in an alternative approach to the many-electron problem in molecules, and is suitable for any courses dealing with computational methods in quantum chemistry.

Many-Electron Densities and Reduced Density Matrices - Jerzy Cioslowski 2012-12-06

Science advances by leaps and bounds rather than linearly in time. I t is not uncommon for a new concept or approach to generate a lot of initial interest, only to enter a quiet period of years or decades and then suddenly reemerge as the focus of new exciting investigations. This is certainly the case of the reduced density matrices (a k a N-matrices or RDMs), whose promise of a great simplification of quantum-chemical approaches faded away when the prospects of formulating the auxil iary yet essential N-representability conditions turned quite bleak. How ever, even during the period that followed this initial disappointment, the 2-matrices and their one-particle counterparts have been ubiquitous in the formalisms of modern electronic structure theory, entering the correlated-level expressions for the first-order response properties, giv ing rise to natural spinorbitals employed in the configuration interaction method and in rigorous analysis of electronic wavefunctions, and al lowing direct calculations of ionization potentials through the extended Koopmans'theorem. The recent research of Nakatsuji, Valdemoro, and Mazziotti her alds a renaissance of the concept of RDlvls that promotes them from the role of interpretive tools and auxiliary quantities to that of central variables of new electron correlation formalisms. Thanks to the economy of information offered by RDMs, these formalisms surpass the conven tional approaches in conciseness and elegance of formulation. As such, they hold the promise of opening an entirely new chapter of quantum chemistry.

New Electron Correlation Methods and their Applications, and Use of Atomic Orbitals with Exponential Asymptotes - 2021-09-24

Advances in Quantum Chemistry presents surveys of current topics in this rapidly developing field one that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry, and biology. It features detailed reviews written by leading international researchers. In this volume the readers are presented with an exciting combination of themes. Presents surveys of current topics in this rapidly-developing field that has emerged at the cross section of the historically established areas of mathematics, physics, chemistry and biology Features detailed reviews written by leading international researchers

Algebraic and Diagrammatic Methods in Many-Fermion Theory - Frank E. Harris 2020-01-15

This text on the use of electron correlation effects in the description of the electronic structure of atoms, molecules, and crystals is intended for graduate students in physical chemistry and physics. Modern theories of electronic structure and methods of incorporating electron correlation contributions are developed using a diagrammatic and algebraic formulation, and the methods developed in the text are illustrated with examples from molecular and solid state quantum mechanics. A brief Introduction is followed by chapters on operator algebra, the independent-particle model, occupation-number formalism, and diagrams. Additional topics include the configuration-interaction method, the many-body perturbation theory, and the coupled-cluster method.

Magnetism: A Synchrotron Radiation Approach - Eric Beaurepaire 2006-08-29

This volume contains the edited lectures of the fourth Mittelwihr school on 'Magnetism and Synchrotron Radiation'. This series of events introduces graduate students and nonspecialists from related disciplines to the field of magnetism and magnetic materials with emphasis on synchrotron radiation as an experimental tool of investigation. These lecture notes present in particular the state of the art regarding the analysis of magnetic properties of new materials.

Rare Earth Element - Jose Edgar Alfonso Orjuela 2017-07-26

Rare earth elements have significant physical and chemical properties, which have been made indispensable in many magnetic, electronic, and optical applications. For instance, rare earth magnets have high magnetic intensity that can be retained at high temperatures, making them ideal for aerospace applications. Moreover, rare earth elements allow to fabricate faster, smaller, and lighter devices such as cell phones and hard drives. They are also important for in-ear headphones, microphones, loudspeakers, optical fibers, smartphones, and tablet computers. All these technological possibilities have made sure that the

rare earth elements are part of the daily life. Therefore, this book has a main objective to let the readers know useful information about the rare earth elements that possibly allow development of the researches in different fields of science where the rare earth elements are used.

Modern Quantum Chemistry - Attila Szabo 2012-06-08

This graduate-level text explains the modern in-depth approaches to the calculation of electronic structure and the properties of molecules. Largely self-contained, it features more than 150 exercises. 1989 edition.

Recent Advances in the Theory of Chemical and Physical Systems - Jean-Pierre Julien 2006-05-05

Advances in the Theory of Chemical and Physical Systems is a collection of 26 selected papers from the scientific presentations made at the 9th European Workshop on Quantum Systems in Chemistry and Physics (QSCP-IX) held at Les Houches, France, in September 2004. This volume encompasses a spectrum of developing topics in which scientists place special emphasis on theoretical methods in the study of chemical and physical properties of various systems: Quantum Chemical Methods (including CC and DFT for excited states) Relativistic and Heavy-Element Systems (including radiative and nuclear effects)Complexes and Clusters (including metal complexes and clusters) Complex Systems (including quasicrystals, nanotubes and proteins).

Brillouin-Wigner Methods for Many-Body Systems - Stephen Wilson 2012-03-01

Brillouin-Wigner Methods for Many-Body Systems gives an introduction to many-body methods in electronic structure theory for the graduate student and post-doctoral researcher. It provides researchers in many-body physics and theoretical chemistry with an account of Brillouin-Wigner methodology as it has been developed in recent years to handle the multireference correlation problem. Moreover, the frontiers of this research field are defined. This volume is of interest to atomic and molecular physicists, physical chemists and chemical physicists, quantum chemists and condensed matter theorists, computational chemists and applied mathematicians.

Hyperspherical Harmonics and Generalized Sturmians - John S. Avery 2002-05-31

This book explores the connections between the theory of hyperspherical harmonics, momentum-space quantum theory, and generalized Sturmian basis functions; and it introduces methods which may be used to solve many-particle problems directly, without the use of the self-consistent-field approximation. The method of many-electron Sturmians offers an interesting and fresh alternative to the usual SCF-CI methods for calculating atomic and molecular structure. When many-electron Sturmians are used, and when the basis potential is chosen to be the attractive potential of the nuclei in the system, the following advantages are offered: the matrix representation of the nuclear attraction potential is diagonal; the kinetic energy term vanishes from the secular equation; the Slater exponents of the atomic orbitals are automatically optimized; convergence is rapid; a correlated solution to the many-electron problem can be obtained directly, without the use of the SCF approximation; and excited states can be obtained with good accuracy.

Quantal Density Functional Theory II - Viraht Sahni 2009-10-16

In my original proposal to Springer for a book on Quantal Density Functional Theory, I had envisaged one that was as complete in its presentation as possible, describing the basic theory as well as the approximation methods and a host of applications. However,after workingon the bookforabout ?ve years, I realizedthat the goal was too ambitious, and that I would be writing for another ?ve years for it to be achieved. Fortunately,there was a natural breakin the material, and I proposed to my editor, Dr. Claus Ascheron, that we split the book into two components: the ?rst on the basic theoretical framework, and the second on approximation methods and applications. Dr. Ascheron consented, and I am thankful to him for agreeing to do so. Hence, we published Quantal Density Functional Theory in 2004, and are now publishing Quantal Density Functional Theory II: Approximation Methods and Applications. One signi?cant advantage of this, as it turns out, is that I have been able to incorporate in each volume the most recent understandings available. This volume, like the earlier one, is aimed at advanced undergraduates in physics and chemistry, graduate students

and researchers in the ?eld. It is written in the same pedagogical style with details of all proofs and numerous ?gures provided to explain the physics. The book is independent of the ?rst volume and stands on its own. However, proofs given in the ?rst volume are not repeated here.

The Symmetric Group in Quantum Chemistry - R. Pauncz 2018-05-04

This is the first book to provide comprehensive treatment of the use of the symmetric group in quantum chemical structures of atoms, molecules, and solids. It begins with the conventional Slater determinant approach and proceeds to the basics of the symmetric group and the construction of spin eigenfunctions. The heart of the book is in the chapter dealing with spin-free quantum chemistry showing the great interpretation value of this method. The last three chapters include the unitary group approach, the symmetric group approach, and the spin-coupled valence bond method. An extensive bibliography concludes the book.

Introductory Quantum Mechanics with MATLAB - James R. Chelikowsky 2018-08-24

Presents a unique approach to grasping the concepts of quantum theory with a focus on atoms, clusters, and crystals Quantum theory of atoms and molecules is vitally important in molecular physics, materials science, nanoscience, solid state physics and many related fields. Introductory Quantum Mechanics with MATLAB is designed to be an accessible guide to quantum theory and its applications. The textbook uses the popular MATLAB programming language for the analytical and numerical solution of quantum mechanical problems, with a particular focus on clusters and assemblies of atoms. The textbook is written by a noted researcher and expert on the topic who introduces density functional theory, variational calculus and other practice-proven methods for the solution of quantum-mechanical problems. This important guide: - Presents the material in a didactical manner to help students grasp the concepts and applications of quantum theory -Covers a wealth of cutting-edge topics such as clusters, nanocrystals, transitions and organic molecules -Offers MATLAB codes to solve real-life quantum mechanical problems Written for master's and PhD students in physics, chemistry, material science, and engineering sciences, Introductory Quantum Mechanics with MATLAB contains an accessible approach to understanding the concepts of quantum theory applied to atoms, clusters, and crystals.

Recent Progress in Coupled Cluster Methods - Petr Cársky 2010-07-26

I feel very honored that I have been asked to write a Foreword to this book. The subject of the book – “Coupled cluster theory” – has been around for about half a century. The basic theory and explicit equations for closed-shell ground states were formulated before 1970. At the beginning of the seventies the rst ab initio calcu- tion were carried out. At that time speed and memory of computers were very limited compared to today’s standards. Moreover, the size of one-electron bases employed was small, so that it was only possible to achieve an orientation in methodical aspects rather than to generate new signi cant results. Extensive use of the coupled-cluster method started at the beginning of the eighties. With the help of more powerful computers the results of coupled-cluster approaches started to yield more and more interesting results of relevance to the interpretation of experimental data. New ideas in methodology kept appearing and computer codes became more and more ef cient. This exciting situation continues to this very day. Remarkably enough, even the - quired equations can now be generated by a computer with the help of symbolic languages. The size of this monograph and the rich variety of articles it contains attests to the usefulness and viability of the couple-cluster formalism for the h- dling of many-electron correlation effects. This represents a vivid testimony of a tremendous work that has been accomplished in coupled-cluster methodology and its exploitation.

Stochastic Approaches to Electron Transport in Micro- and Nanostructures - Mihail Nedjalkov 2021-04-05

The book serves as a synergistic link between the development of mathematical models and the emergence of stochastic (Monte Carlo) methods applied for the simulation of current transport in electronic devices. Regarding the models, the historical evolution path, beginning

from the classical charge carrier transport models for microelectronics to current quantum-based nanoelectronics, is explicatively followed. Accordingly, the solution methods are elucidated from the early phenomenological single particle algorithms applicable for stationary homogeneous physical conditions up to the complex algorithms required for quantum transport, based on particle generation and annihilation. The book fills the gap between monographs focusing on the development of the theory and the physical aspects of models, their application, and their solution methods and monographs dealing with the purely theoretical approaches for finding stochastic solutions of Fredholm integral equations.

Handbook of Theoretical Atomic Physics - Miron Amusia 2012-07-23
The aim of this book is to present highly accurate and extensive theoretical Atomic data and to give a survey of selected calculational methods for atomic physics, used to obtain these data. The book presents the results of calculations of cross sections and probabilities of a broad variety of atomic processes with participation of photons and electrons, namely on photoabsorption, electron scattering and accompanying effects. Included are data for photoabsorption and electron scattering cross-sections and probabilities of vacancy decay formed for a large number of atoms and ions. Attention is also given to photoionization and vacancy decay in endohedrals and to positron-atom scattering. The book is richly illustrated. The methods used are one-electron Hartree-Fock and the technique of Feynman diagrams that permits to include many-electron correlations. This is done in the frames of the Random Phase approximation with exchange and the many-body perturbation theory. Newly obtained and previously collected atomic data are presented. The atomic data are useful for investigating the electronic structure and physical processes in solids and liquids, molecules and clusters, astronomical objects, solar and planet atmospheres and atomic nucleus. Deep understanding of chemical reactions and processes is reached by deep and accurate knowledge of atomic structure and processes with participation of atoms. This book is useful for theorists performing research in different domains of contemporary physics, chemistry and biology, technologists working on production of new materials and for experimentalists performing research in the field of photon and electron interaction with atoms, molecules, solid bodies and liquids.

Chemometrics and Cheminformatics in Aquatic Toxicology - Kunal Roy 2022-01-06
CHEMOMETRICS AND CHEMINFORMATICS IN AQUATIC TOXICOLOGY Explore chemometric and cheminformatic techniques and tools in aquatic toxicology Chemometrics and Cheminformatics in Aquatic Toxicology delivers an exploration of the existing and emerging problems of contamination of the aquatic environment through various metal and organic pollutants, including industrial chemicals, pharmaceuticals, cosmetics, biocides, nanomaterials, pesticides, surfactants, dyes, and more. The book discusses different chemometric and cheminformatic tools for non-experts and their application to the analysis and modeling of toxicity data of chemicals to various aquatic organisms. You'll learn about a variety of aquatic toxicity databases and chemometric software tools and webservers as well as practical examples of model development, including illustrations. You'll also find case studies and literature reports to round out your understanding of the subject. Finally, you'll learn about tools and protocols including machine learning, data mining, and QSAR and ligand-based chemical design methods. Readers will also benefit from the inclusion of: A thorough introduction to chemometric and cheminformatic tools and techniques, including machine learning and data mining An exploration of aquatic toxicity databases, chemometric software tools, and webservers Practical examples and case studies to highlight and illustrate the concepts contained within the book A concise treatment of chemometric and cheminformatic tools and their application to the analysis and modeling of toxicity data Perfect for researchers and students in chemistry and the environmental and pharmaceutical sciences, Chemometrics and Cheminformatics in Aquatic Toxicology will also earn a place in the libraries of professionals in the chemical industry and regulators whose work involves chemometrics.

Many-Body Methods in Chemistry and Physics - Isaiah Shavitt

2009-08-06
This book describes the mathematical and diagrammatic techniques employed in the popular many-body methods to determine molecular structure, properties and interactions.
Quantum Systems in Chemistry and Physics. Trends in Methods and Applications - R. McWeeny 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.
Many-Electron Approaches in Physics, Chemistry and Mathematics - Volker Bach 2014-07-17
This book provides a broad description of the development and (computational) application of many-electron approaches from a multidisciplinary perspective. In the context of studying many-electron systems Computer Science, Chemistry, Mathematics and Physics are all intimately interconnected. However, beyond a handful of communities working at the interface between these disciplines, there is still a marked separation of subjects. This book seeks to offer a common platform for possible exchanges between the various fields and to introduce the reader to perspectives for potential further developments across the disciplines. The rapid advances of modern technology will inevitably require substantial improvements in the approaches currently used, which will in turn make exchanges between disciplines indispensable. In essence this book is one of the very first attempts at an interdisciplinary approach to the many-electron problem.
Representing Electrons - Theodore Arabatzis 2006
Both a history and a metahistory, Representing Electrons focuses on the development of various theoretical representations of electrons from the late 1890s to 1925 and the methodological problems associated with writing about unobservable scientific entities. Using the electron—or rather its representation—as a historical actor, Theodore Arabatzis illustrates the emergence and gradual consolidation of its representation in physics, its career throughout old quantum theory, and its appropriation and reinterpretation by chemists. As Arabatzis develops this novel biographical approach, he portrays scientific representations as partly autonomous agents with lives of their own. Furthermore, he argues that the considerable variance in the representation of the electron does not undermine its stable identity or existence. Raising philosophical issues of contentious debate in the history and philosophy of science—namely, scientific realism and meaning change—Arabatzis addresses the history of the electron across disciplines, integrating historical narrative with philosophical analysis in a book that will be a touchstone for historians and philosophers of science and scientists alike.
Interacting Electrons - Richard M. Martin 2016-06-30
Recent progress in the theory and computation of electronic structure is bringing an unprecedented level of capability for research. Many-body methods are becoming essential tools vital for quantitative calculations and understanding materials phenomena in physics, chemistry, materials science and other fields. This book provides a unified exposition of the most-used tools: many-body perturbation theory, dynamical mean field theory and quantum Monte Carlo simulations. Each topic is introduced with a less technical overview for a broad readership, followed by in-depth descriptions and mathematical formulation. Practical guidelines, illustrations and exercises are chosen to enable readers to appreciate the complementary approaches, their relationships, and the advantages and disadvantages of each method. This book is designed for graduate

students and researchers who want to use and understand these advanced computational tools, get a broad overview, and acquire a basis for participating in new developments.

Advances in Chemical Physics - Ilya Prigogine 2009-09-08

The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical, authoritative evaluations of advances in every area of the discipline. Filled with cutting-edge research reported in a cohesive manner not found elsewhere in the literature, each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics.

Many-body Approaches at Different Scales - G.G.N Angilella 2018-03-24

This book presents a collection of invited research and review contributions on recent advances in (mainly) theoretical condensed matter physics, theoretical chemistry, and theoretical physics. The volume celebrates the 90th birthday of N.H. March (Emeritus Professor, Oxford University, UK), a prominent figure in all of these fields. Given the broad range of interests in the research activity of Professor March, who collaborated with a number of eminent scientists in physics and chemistry, the volume embraces quite diverse topics in physics and chemistry, at various dimensions and energy scales. One thread connecting all these topics is correlation in aggregated states of matter, ranging from nuclear physics to molecules, clusters, disordered condensed phases such as the liquid state, and solid state physics, and the various phase transitions, both structural and electronic, occurring therein. A final chapter leaps to an even larger scale of matter aggregation, namely the universe and gravitation. A further no less important common thread is methodological, with the application of theoretical physics and chemistry, particularly density functional theory and statistical field theory, to both nuclear and condensed matter.

Progress in Physical Chemistry Volume 3 - Franz Michael Dolg 2010-01-01

Progress in Physical Chemistry is a collection of recent »Review Articles« published in the »Zeitschrift für Physikalische Chemie«. The third volume of the series "Progress in Physical Chemistry" comprises 27 articles, most of them with review character, written by the members of the Priority Program (SPP) 1145 of the German Research Foundation (DFG).

Modern and Universal First-principles Methods for Many-electron Systems in Chemistry and Physics - Michael Dolg 2010