Relativistic Quantum Theory Of Atoms And Molecules Theory And Computation Springer Series On Atomic Optical And Plasma Physics

This book gives an introduction to quantum mechanics with the matrix method. Heisenberg's matrix mechanics is described in detail. The fundamental equations are derived by algebraic methods using matrix calculus. Only a brief description of Schrödinger's wave mechanics is given (in most books exclusively treated), to show their equivalence to Heisenberg's matrix method. In the first part the historical development of Quantum theory by Planck, Bohr and Sommerfeld is sketched, followed by the ideas and methods of Heisenberg, Born and Jordan. Then Pauli's spin and exclusion principles are treated. Pauli's exclusion principle leads to the structure of atoms. Finally, Dirac ?s relativistic quantum mechanics is shortly presented. Matrices and matrix equations are today easy to handle when implementing numerical algorithms using standard software as MAPLE and Mathematica.

From the reviews: "The text is almost self-contained and requires only an elementary knowledge of probability theory at the graduate level. The book under review is recommended to mathematicians, physicists and graduate students interested in mathematical physics and stochastic processes. Furthermore, some selected chapters can be used as sub-textbooks for advanced courses on stochastic processes, quantum theory and quantum chemistry." ZAA

This book is primarily intended for graduate chemists and chemical physicists. Indeed, it is based on a graduate course that I give in the Chemistry Depart ment of Southampton University. Nowadays undergraduate chemistry courses usually include an introduction to quantum mechanics with particular reference to molecular properties and there are a number of excellent textbooks aimed specifically at undergraduate chemists. In valence theory and molecular spectroscopy physical concepts are often encountered that are normally taken on trust. For example, electron spin and the anomalous magnetic moment of the electron are usually accepted as postulates, although they are well understood by physicists. In addition, the advent of new techniques has led to experimental situations that can only be accounted for adequately by relatively sophisticated physical theory. Relativis tic corrections to molecular orbital energies are needed to explain X-ray photo electron spectra, while the use oflasers can give rise to multiphoton transitions, which are not easy to understand using the classical theory of radiation. Of course, the relevant equations may be extracted from the literature, but, if the underlying physics is not understood, this is a practice that is at best dissatisfy ing and at worst dangerous. One instance where great care must be taken is in the use of spectroscopically determined parameters to test the accuracy of elec tronic wave functions.

What exactly did Einstein do that's so important in physics? We provide an introduction to his physics at a level accessible to an undergraduate student. All equations are worked out in detail from the beginning. Although the book is written with primarily a physics readership in mind (it can also function as a textbook), enough pedagogical support material is provided that anyone with a solid background in introductory physics (say, an engineer) can, with someeffort, understand a good part this presentation.We show why Einstein's papers were decisive to our understanding of matter as composed of molecules and atoms; why is he regarded as a foundingfather of quantum theory; how did his relativity theory bring about the new understanding that time, just like space, is relative; and how did his general relativity extend Newton's theory to new physical realm, allowing us to study black holes and cosmology.

This graduate text introduces relativistic quantum theory, emphasising its important applications in condensed matter physics. Relativistic quantum theory is the unification into a consistent theory of Einstein's theory of relativity and the quantum mechanics of Bohr, Schrödinger, and Heisenberg, etc. Beginning with basic theory, the book then describes essential topics. Many worked examples and exercises are included along with an extensive reference list. This clear account of a crucial topic in science will be valuable to graduates and researchers working in condensed matter physics and quantum physics.

This first volume of this two-volume set deals with the important recent discovery of the photomagneton of electromagnetic radiation, a discovery which is fundamental in quantum field theory and in quantum mechanics in matter. The photomagneton is the elementary quantum of magnetic flux density carried by the individual photon in free space, and is generated directly by the intrinsic angular momentum of the free photon. The volume develops the theory of the photomagneton in a series of papers, which cover all the major aspects of the theory, from classical electrodynamics to the relativistic quantum field. Several suggestions are given for experimental tests, and the available experimental evidence is discussed in detail. The overall conclusion of the series of papers is that the photomagneton, which is observable experimentally in magneto-optical phenomena, indicates the presence in free space of a novel, longitudinal, magnetic flux density, linked ineluctably to the usual transverse components. If the photomagneton is not observed, then a paradox would have emerged at the most fundamental electrodynamical level, necessitating a modification of the Maxwell equations themselves. Contents:The Photon has Three PolarizationsThe Photomagneton B(3) and Longitudinal Ghost Field B(3) of ElectromagnetismThe Relation between Transverse and Longitudinal Solutions of Maxwell's EquationsThe One Electron Inverse Faraday Effect: The Role of the Equivalent Magnetic Field B(3)Longitudinal Solutions of Maxwell's Equations in the Lorentz Gauge in Free SpaceIrreducible Tensorial Representations in R(3) of the Longitudinal Ghost Fields of Free Space ElectromagnetismTheory of the Optical Faraday EffectClassical Relativistic Theory of the Longitudinal Ghost Fields of ElectromagnetismThe Magnetic Fields and Rotation Generators of Free Space ElectromagnetismSome Consequences of Finite Photon Mass in Electromagnetic TheoryQuestions about the Field B(3)Molecular Theory of Optical NMR Spectroscopy: Light Induced Bulk and Site Specific ShiftsOptical NMR as a Shielding PhenomenonManifestly Covariant Theory of the Electromagnetic Field: Longitudinal Magnetic Fields in Non-Conducting and Conducting Media, Reflection and RefractionCriticisms of the Diagrammatic Approach to Complete

Experiment SymmetryThe Photon's Magnetostatic Flux Quantum: Its Role in Circular Dichroism and the Electrical Kerr EffectThe Maxwellian Limit of the Einstein-DeBroglie Theory of Electromagnetic RadiationAppendices Readership: Optical physicists, spectroscopists, cosmologists and field theoreticians. keywords:

When one approaches the study of the quantal relativistic theory of the electron, one may be surprised by the gap which lies between the frame of the experiments, i.e. the real geometry of the space and time, and the abstraction of the complex matrices and spinors formalism employed in the presentation of the theory. This book uses a theory of the electron, introduced by David Hestenes, in which the mathematical language is the same as the one of the geometry of the space and time. Such a language not only allows one to find again the well known results concerning the one-electron atoms theory but furthermore leads easily to the resolution of problems considered for a long time without solution.

The first volume of this two part series is concerned with the fundamental aspects of relativistic quantum theory, outlining the enormous progress made in the last twenty years in this field. The aim was to create a book such that researchers who become interested in this exciting new field find it useful as a textbook, and do not have to rely on a rather large number of specialized papers published in this area. · No title is currently available that deals with new developments in relativistic quantum electronic structure theory · Interesting and relevant to graduate students in chemistry and physics as well as to all researchers in the field of quantum chemistry · As treatment of heavy elements becomes more important, there will be a constant demand for this title

Continuing the exceptional tradition of the previous editions, Quantum Mechanics, Fourth Edition provides essential information about atomic and subatomic systems and covers some modern applications of the field. Supported by a Web page that contains a bibliography, color versions of some of the illustrations, and links to other relevant sites, the book shows how cutting-edge research topics of quantum mechanics have been applied to various disciplines. It first demonstrates how to obtain a wave equation whose solutions determine the energy levels of bound systems. The theory is then made more general and applied to a number of physical examples. Later chapters describe the connection between relativity and quantum mechanics, give some examples of how quantum mechanics has been used in information processing, and, finally, discuss the conceptual and philosophical implications of the subject. New to the Fourth Edition: A chapter on quantum information processing that includes applications to the encryption and de-encryption of coded messages A chapter on relativistic quantum mechanics and introductory quantum field theory Updated material on the conceptual foundations of quantum physics containing discussions of non-locality, hidden variables, and parallel universes Expanded information on tunneling microscopy and the Bose-Einstein condensate Presenting up-to-date information on the conceptual and philosophical aspects of quantum mechanics, this revised edition is suitable both for undergraduates studying physics, chemistry, or mathematics and for researchers involved in quantum physics.

Advanced Quantum Theory is a concised, comprehensive, well-organized text based on the techniques used in theoretical elementary particle physics and extended to other branches of modern physics as well. While it is especially valuable reading for students and professors of physics, a less cursory survey should aid the nonspecialist in mastering the principles and calculational tools that probe the quantum nature of the fundamental forces. The initial application is to nonrelativistic scattering graphs encountered in atomic, solid state, and nuclear physics. Then, focusing on relativistic Feynman Diagrams and their construction in lowest order -- applied to electromagnetic, strong, weak, and gravitational interactions -- this bestseller also covers relativistic quantum theory based on group theoretical language, scattering theory, and finite parts of higher order graphs. This new edition includes two chapters on the quark model at low energies.

A sequel to the well received book, Quantum Mechanics by T Y Wu, this book carries on where the earlier volume ends. This present volume follows the generally pedagogic style of Quantum Mechanics. The scope ranges from relativistic quantum mechanics to an introduction to quantum field theory with quantum electrodynamics as the basic example and ends with an exposition of important issues related to the standard model. The book presents the subject in basic and easy-to-grasp notions which will enhance the purpose of this book as a useful textbook in the area of relativistic quantum mechanics and quantum electrodynamics.

This book presents new aspects of quantum electrodynamics (QED), a quantum theory of photons with electrons, from basic physics to physical chemistry with mathematical rigor. Topics covered include spin dynamics, chemical reactivity, the dual Cauchy problem, and more. Readers interested in modern applications of quantum field theory in nano-, bio-, and open systems will enjoy learning how the up-to-date quantum theory of radiation with matter works in the world of QED. In particular, chemical ideas restricted now to nonrelativistic quantum theory are shown to be unified and extended to relativistic quantum field theory that is basic to particle physics and cosmology: realization of the new-generation quantum theory. Readers are assumed to have a background equivalent to an undergraduate student's elementary knowledge in electromagnetism, quantum mechanics, chemistry, and mathematics.

This advanced textbook supplies graduate students with a primer in quantum theory. A variety of processes are discussed with concepts such as potentials, classical current distributions, prescribed external fields dealt with in the framework of relativistic quantum mechanics. Then, in an introduction to field theory, the author emphasizes the deduction of the said potentials or currents. A modern presentation of the subject together with many exercises, unique in its unusual underlying concept of combining relativistic quantum mechanics with basic quantum field theory.

In this book, quantum mechanics is developed from the outset on a relativistic basis, using the superposition principle, Lorentz invariance and gauge invariance. Nonrelativistic quantum mechanics appears as a special case, and classical relativistic mechanics as another one. These special cases are important for giving plausible names to operators, for example "orbital angular momentum", "spin" or "magnetic moment". A subject which is treated for the first time in this book is the theory of binaries in terms of differential equations which have the mathematical structure of the corresponding one-body equations (Klein--Gordon for two spin- less particles, Dirac for two spinor particles).

This book provides an introduction to the essentials of relativistic effects in quantum chemistry, and a reference work that collects all the major developments in this field. It is designed for the graduate student and the computational chemist with a good background in nonrelativistic theory. In addition to explaining the necessary theory in detail, at a level that the non-expert and the student should readily be able to follow, the book discusses the implementation of the theory and practicalities of its use in calculations. After a brief introduction to classical relativity and electromagnetism, the Dirac equation is presented, and its symmetry, atomic solutions, and interpretation are explored.

Four-component molecular methods are then developed: self-consistent field theory and the use of basis sets, double-group and time-reversal symmetry, correlation methods, molecular properties, and an overview of relativistic density functional theory. The emphases in this section are on the basics of relativistic theory and how relativistic theory differs from nonrelativistic theory. Approximate methods are treated next, starting with spin separation in the Dirac equation, and proceeding to the Foldy-Wouthuysen, Douglas-Kroll, and related transformations, Breit-Pauli and direct perturbation theory, regular approximations, matrix approximations, and pseudopotential and model potential methods. For each of these approximations, one-electron operators and many-electron methods are developed, spin-free and spin-orbit operators are presented, and the calculation of electric and magnetic properties is discussed. The treatment of spin-orbit effects with correlation rounds off the presentation of approximate methods. The book concludes with a discussion of the qualitative changes in the picture of structure and bonding that arise from the inclusion of relativity.

Heavy atoms and their compounds are important in many areas of modern technology. Their versatility in the reactions they undergo is the reason that they can be found in most homogeneous and heterogeneous catalysts. Their magnetism is the decisive property that qualifies them as materials for modern storage devices. The phenomena observed in compounds of heavy atoms such as phosphorescence, magnetism or the tendency for high valency in chemical reactions can to a large extent be traced back to relativistic effects in their electronic structure. Thus, in many respects relativistic effects dominate the physics and chemistry of heavy atoms and their compounds. Chemists are usually aware of these phenomena. However, the theory behind them is not part of the standard chemistry curriculum and thus not widely known among experimentalists. Whilst the relativistic quantum theory of electronic structure is well established in physics, applications of the theory to chemical systems and materials have been feasible only in the last decade and their practical applications in connection with chemical experiment is somewhat out of sight of modern theoretical physics. Relativistic Effects in Heavy Element Chemistry and Physics intends to bridge the gap between chemistry and physics on the one hand and theory and experiment on the other. Topics covered include: - A broad range from quantum electrodynamics to the phenomenology of the compounds of heavy and superheavy elements; - A state-of-the-art survey of the most important theoretical developments and applications in the field of relativistic effects in heavy-element chemistry and physics in the last decade; - Special emphasis on the work of researchers in Europe and Germany in the framework of research programmes of the European Science Foundation and the German Science Foundation.

Atomic physics and its underlying quantum theory are the point of departure for many modern areas of physics, astrophysics, chemistry, biology, and even electrical engineering. This textbook provides a careful and eminently readable introduction to the results and methods of empirical atomic physics. The student will acquire the tools of quantum physics and at the same time learn about the interplay between experiment and theory. A chapter on the quantum theory of the chemical bond provides the reader with an introduction to molecular physics. Plenty of problems are given to elucidate the material. The authors also discuss laser physics and nonlinear spectroscopy, incorporating latest experimental results and showing their relevance to basic research. Extra items in the second edition include solutions to the exercises, derivations of the relativistic Klein-Gordon and Dirac equations, a detailed theoretical derivation of the Lamb shift, a discussion of new developments in the spectroscopy of inner shells, and new applications of NMR spectroscopy, for instance tomography.

The field of relativistic electronic structure theory is generally not part of theoretical chemistry education, and is therefore not covered in most quantum chemistry textbooks. This is due to the fact that only in the last two decades have we learned about the importance of relativistic effects in the chemistry of heavy and superheavy elements. Developments in computer hardware together with sophisticated computer algorithms make it now possible to perform four-component relativistic calculations for larger molecules. Two-component and scalar all-electron relativistic schemes are also becoming part of standard ab-initio and density functional program packages for molecules and the solid state. The second volume of this two-part book series is therefore devoted to applications in this area of quantum chemistry and physics of atoms, molecules and the solid state. Part 1 was devoted to fundamental aspects of relativistic electronic structure theory whereas Part 2 covers more of the applications side. This volume opens with a section on the Chemistry of the Superheavy Elements and contains chapters dealing with Accurate Relativistic Fock-Space Calculations for Many-Electron Atoms, Accurate Relativistic Calculations Including QED, Parity-Violation Effects in Molecules, Accurate Determination of Electric Field Gradients for Heavy Atoms and Molecules, Two-Component Relativistic Effective Core Potential Calculations for Molecules, Relativistic Ab-Initio Model Potential Calculations for Molecules and Embedded Clusters, Relativistic Pseudopotential Calculations for Electronic Excited States, Relativistic Effects on NMR Chemical Shifts, Relativistic Density Functional Calculations on Small Molecules, Quantum Chemistry with the Douglas-Kroll-Hess Approach to Relativistic Density Functional Theory, and Relativistic Solid State Calculations. - Comprehensive publication which focuses on new developments in relativistic quantum electronic structure theory - Many leaders from the field of theoretical chemistry have contributed to the TCC series - Will no doubt become a standard text for scientists in this field.

During the last two decades the explorations of di?erent processes accom- nyingion–atom collisions athigh-impactenergieshavebeenasubjectofmuch interest. This interest was generated not only by the advent of accelerators of relativistic heavy ions which enabled one to investigate these collisions in an experiment and possible applications of obtained results in other ?elds of physics, but also by the variety of physical mechanisms underlying the atomic collisional phenomena at high impact energies. Often highly charged projectiles produced at accelerators of heavy ions are not fully stripped ions but carry one or more very tightly bound el- trons. In collisions with atomic targets, these electrons can be excited or lost and this may occur simultaneously with electronic transitions in the target. The present book concentrates on, and may serve as an introduction to, th- retical methods which are used to describe the projectile–electron transitions occurringinhigh-energycollisionsbetweenionsandneutralatoms.Special- tention is given to relativistic impact energies and highly charged projectiles. Experimental results are used merely as illustrations and tests for theory. This book will be useful to graduate students and professional scientists who are interested in studying atomic collisions occurring at high-impact - ergies. It assumes that the reader possesses the basic knowledge in classical electrodynamics and nonrelativistic and relativistic quantum mechanics.

Relativistic effects are of major importance for understanding the properties of heavier atoms and molecules. Volumes I-III of Relativistic Theory of Atoms and Molecules constitute the only available bibliography on related calculations. In Volume III, 3792 new references covering 1993-1999 are added to the database. The material is characterized by an analysis of the respective papers. The volume gives the user a comprehensive bibliography on relativistic atomic and molecular calculations, including studies on the Dirac equation and related solid-state work.

This handbook covers new methodological developments and applications of relativistic quantum chemistry. It also pays attention to the foundation of relativistic quantum mechanics and addresses a number of fundamental issues that have not been covered by any book. For instance, what is the appropriate relativistic many-electron Hamiltonian? How to do relativistic explicit/local correlation? How to formulate relativistic properties? How to combine double-group and time-reversal symmetries? How to do QED calculations for molecules? Just to name a few. This book aims to establish the big picture of relativistic molecular quantum mechanics, ranging from pedagogic introduction for uninitiated readers, advanced methodologies and efficient algorithms for experts, to possible future perspectives, such that the reader knows when/how to apply/develop the methodologies. This self-contained two-volume book can be regarded as a supplement to the three-volume "Handbook of Computational Chemistry", which contains no relativity at all. It is to be composed of 6 sections with different chapters (will be further expanded), each of which is to be written by the most active experts, who will be invited upon approval of this proposal.

Unlike most introductory and advanced books on quantum mechanics, this book covers a large number of applications of quantum mechanics including their relativistic generalization and even quantum chemistry. It thereby closes a gap between books of quantum mechanics and quantum field theory. Starting with quantum mechanics, the book then treats the equations of relativistic quantum mechanics with emphasis on Dirac's equation, followed by a discussion of spin to finally arrive at quantum field theory. The relativistic equations are used as a starting point to explain all the small corrections to quantum mechanics leading to measurable effects. The chapters on scattering and bound states convey a deep understanding of the field. Hyperfine shifts and dispersive effects like the Lambshift are treated in a comprehensible manner. The beautiful symmetries on which the particle classifications are based are discussed in subsequent sections. The appendices illustrate technical difficulties encountered in calculations. In the third edition of this successful text, published posthumously, many sections have been revised and widely extended. In particular the discussion of Hyperfine shifts, radiation, dispersive effects, quarks have been thoroughly revisited and split up into three chapters. Sections on Kramer's equation and on electroweak interactions have been added. The book will be of interest to researchers and graduate students in quantum mechanics and quantum field theory.

The second edition of Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science expands on some of the latest developments in this fascinating field. The text retains its clear and consistent style, allowing for a readily accessible overview of the complex topic. It is also self-contained, building on the fundamental equations and providing the mathematical background necessary. While some parts of the text have been restructured for the sake of clarity a significant amount of new content has also been added. This includes, for example, an in-depth discussion of the Brown-Ravenhall disease, of spin in current-density functional theory, and of exact two-component methods and its local variants. A strength of the first edition of this textbook was its list of almost 1000 references to the original research literature, which has made it a valuable reference also for experts in the field.

Geared toward research students in physics and chemistry, this text introduces the three main uses of group theory in quantum mechanics: (1) to label energy levels and the corresponding eigenstates; (2) to discuss qualitatively the splitting of energy levels, starting from an approximate Hamiltonian and adding correction terms; and (3) to aid in the evaluation of matrix elements of all kinds. "The theme," states author Volker Heine, "is to show how all this is achieved by considering the symmetry properties of the Hamiltonian and the way in which these symmetries are reflected in the wave functions." Early chapters cover symmetry transformations, the quantum theory of a free atom, and the representations of finite groups. Subsequent chapters address the structure and vibrations of molecules, solid state physics, nuclear physics, and relativistic quantum mechanics. A previous course in quantum theory is necessary, but the relevant matrix algebra appears in an appendix. A series of examples of varying levels of difficulty follows each chapter. They include simple drills related to preceding material as well as extensions of theory and further applications. The text is enhanced with 46 illustrations and 12 helpful appendixes.

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: Dirac's 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.

This book is a distillation of Prof T Y Wu's fifty years of experience teaching quantum theory to many generations of physicists. Starting with chapters on classical physics and the old quantum theory, Prof Wu quickly develops Heisenberg's matrix mechanics and the Schroedinger equation. After a detailed treatment of the general formulation of quantum theory, standard discussions on Perturbation Theory and the Hydrogen Atom follow. A fairly exhaustive treatment of the Zeeman effect is to be found in these chapter. Many electron atoms are treated expertly. The former is treated with great depth; the latter is a good introduction to the subject.

An understanding of the collisions between micro particles is of great importance for the number of fields belonging to physics, chemistry, astrophysics, biophysics etc. The present book, a theory for electron-atom and molecule collisions is developed using non-relativistic quantum mechanics in a systematic and lucid manner. The scattering theory is an essential part of the quantum mechanics course of all universities. During the last 30 years, the author has lectured on the topics presented in this book (collisions physics, photon-atom collisions, electron-atom and electron-molecule collisions, "electron-photon delayed coincidence technique", etc.) at many institutions including Wayne State University, Detroit, MI, The University of Western Ontario, Canada, and The Meerut University, India. The present book is the outcome of those lectures and is written to serve as a textbook for post-graduate and pre-PhD students and as a reference book for researchers.

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Photons and Atoms Photons and Atoms: Introduction to Quantum Electrodynamics provides the necessary background to understand the various physical processes associated with photon-atom interactions. It starts with elementary quantum theory and classical electrodynamics and progresses to more advanced approaches. A critical comparison is made between these different, although equivalent, formulations of quantum electrodynamics. Using this format, the reader is offered a gradual, yet flexible introduction to quantum electrodynamics, avoiding formal discussions and excessive shortcuts. Complementing each chapter are numerous examples and exercises that can be used independently from the rest of the book to extend each chapter in many disciplines depending on the interests and needs of the reader.

Quantum theory as a scientific revolution profoundly influenced human thought about the universe and governed forces of nature. Quantum mechanics is the branch of physics relating to the very small. It results in what may appear to be some very strange conclusions about the physical world. At the scale of atoms and electrons, many of the equations of classical mechanics, which describe how things move at everyday sizes and speeds, cease to be useful. Quantum mechanics (QM) developed over many decades, beginning as a set of controversial mathematical explanations of experiments that the math of classical mechanics could not explain. It began at the turn of the 20th century, around the same time that Albert Einstein published his theory of relativity, a separate mathematical revolution in physics that describes the motion of things at high speeds. Quantum mechanics attempts to describe and account for the properties of molecules and atoms and their constituents--electrons, protons, neutrons, and other more esoteric particles such as quarks and gluons. These properties include the interactions of the particles with one another and with electromagnetic radiation. An essential feature of quantum mechanics is that it is generally impossible, even in principle, to measure a system without disturbing it; the detailed nature of this disturbance and the exact point at which it occurs are obscure and controversial. Theoretical Concepts of Quantum Mechanics represents a rich account of foundation, scientific history of quantum mechanics, relativistic quantum mechanics and field theory, and different methods to solve the Schrodinger equation. This book will be of valuable for students and researchers.

This book is intended for physicists and chemists who need to understand the theory of atomic and molecular structure and processes, and who wish to apply the theory to practical problems. As far as practicable, the book provides a self-contained account of the theory of relativistic atomic and molecular structure, based on the accepted formalism of bound-state Quantum Electrodynamics. The author was elected a Fellow of the Royal Society of London in 1992.

The material contained in this work concerns relativistic quantum mechanics, and as such pertains to classical fields. On the one hand it is meant to serve as a text on the subject, a desire stemming from the author's fruitless searches for an adequate, up-to-date reference when lecturing on these topics. At times the supplementary material was found to exceed by far that in the assigned text. On the other hand, there is some flavor of a monograph to what follows, most particularly in the later chapters, for a major goal is to demonstrate just how far we can advance our understanding of the behavior of stable particles and their interactions without introducing quantized fields. Those wishing to describe the world in this way may view the result as a point of departure, despite the fact that their wish remains unfulfilled. Confirmed quantum-field theorists, however, will doubtless view it as a summary of just why they feel compelled to quantize the fields. Approximately half the book is devoted to the single-particle Dirac equation and its solutions. A great deal of detail is provided in this respect, and the discus sion is reasonably comprehensive. The Dirac equation is extraordinarily important in its own right, particularly as a basis for quantum electrodynamics (QED), and is thus worthy of extensive study.

This volume contains all of the invited lectures presented at the NATO ARWon "New Methods in Quantum Theory" held in Halkidiki, Greece from May 14th to May 19th, 1995. This survey of new perspectives, techniques and results in quantum theory contains 26 chapters by leading quantum chemists and physicists from 14 countries. The book covers a wide range of topics, though the emphasis throughout is on new approaches and their interrelationships. Topics covered include dimensional scaling, the hyperspherical method applied both to reactive scattering theory and to bound state problems, chaotic behaviour, large-order perturbation theory, complex eigenvalues and quasistationary states, semiclassical methods, cusps in hyperaccurate wave functions, density functional theory, relativistic quantum theory, and quantum Monte Carlo methods. I hope very much that the various lectures presented at this Advanced Research Workshop will be of as great interest to the reader as they were to the participants. The organization of the ARW would have been impossible without the generous funding by NATO, which is gratefully acknowledged. I sincerely thank Drs. J. -M. Cadiou, Assistant Secretary General for Scientific and Environmental Affairs, and J. A. Rausell-Colom, Programme Director for Priority Area on High Technology, North Atlantic Treaty Organization, who helped me throughout the various stages of the ARW.

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.

Thisvolume isdevotedtomethodsfor thestudyoftheeffectsofrelativity on theelectronicstructure ofatomsand molecules. The accurate descrip tionofrelativisticeffectsinheavyatomshaslongbeenrecognizedasoneof the central problems ofatomic physics. Contemporary relativistic atomic structure calculations can be performed almost routinely. Recent years have seen agrowinginterestin thestudyoftheeffects ofrelativityon the structureofmolecules. Even for molecularsystemscontainingatoms from thesecondrowoftheperiodictable theenergyassociatedwith relativistic effects is often larger than that arising from electron correlation. For moleculescontainingheavieratoms relativistic effects become increasingly important, andforsystemscontainingveryheavyatomsrelativityisknown todominatemanychemicalproperties. In this volum, one of the pioneers of relativistic atomic structure calculations, Ian P. Grant, providesadetailedsurveyofthecomputational techniquesemployedincontemporarystudiesoftheeffectsofrelativityon atomicstructure. Thisisanareaofresearchinwhichcalculationscanoften lead to a particularly impressive degreeofagreement between theoryand experiment. Furthermore, theseatomicstudies haveprovided manyofthe foundations of a fully relativistic quantum chemistry. However, the spherical symmetry ofatoms allows significantsimplificationsto bemade in their quantum mechanical treatment, simplifications which are not possibleinstudiesofmolecules. Inparticular, as is wellknown from non relativistictheoriesofmolecularelectronicstructure, itisalmostobligatory to invoke the algebraic approximation in molecular work and use finite basis set expansions. The problem of describing relativistic effects in molecules is addressed in Chapter2 by Stephen Wilson. This chapter is devotedtoab initiorelativisticmolecularstructurecalculationsinwhichall electrons are explicitly considered. The problem of induding relativistic effects in molecular studies is also addressed in Chapters3 and 4. In Chapter 3, Odd Gropen describes the use of relativistic effective core ix x Preface potentials in calculations on molecular systems involving heavy atoms. This approach can lead to more tractable algorithms than the methods described in Chapter2 and thus significantly extends the range of applications. The use of semiempirical methods has yielded a wealth of informationabouttheinfluenceofrelativityonthechemistryoftheheavier elements. Thisimportantarea is reviewed inChapter4 by Pekka Pyykk6. Finally, inChapter5, Harry M."