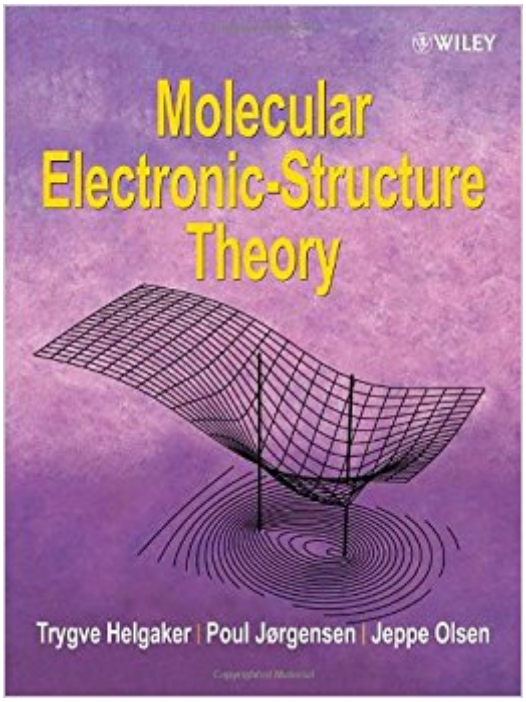
Molecular Electronic-Structure Theory



Synopsis

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.

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Customer Reviews

..."The book affords a profound knowledge of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) "It is the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen and should be available to all students and researchers" (Physics Today, December 2001)..."The book affords a profound knowledge of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) ..."the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basis of...molecular electronic structure methods." (Physics Today, December 2001).,."The book affords a profound knowledge of basic quantum mechanics..." (Jnl of Solid State Electrochemistry, June 2002) .,."the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basis of...molecular electronic structure methods." (Physics Today, December 2001).,."the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basis of...molecular electronic structure methods." (Physics Today, December 2001)."..the most complete and satisfying presentation of the actual armament involved in the computational approach to electronic structure that I have seen, and should be available to all students and researchers who wish to understand the basis of...molecular electronic structure methods." (Physics Today, December 2001)

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single- and multi-configuration states Linear-scaling techniques and the fast multiple method Explicitly correlated wave functions Basis-set convergence and extrapolation Calibration and benchmarking of computational methods, with applications to molecular equilibrium structures, 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.

For a text this thorough and updated, I'd expect a price tag of $150 US or more. It is still not cheap and as a recent edition there are few used ones around, but is a wonderful value for the price given its uniqueness. And don't wait for used copies-- despite the publisher's hype this is NOT an undergrad level text, so those who do buy this will likely end up keeping it as a very fine reference (1,000 pages!) to refer to again and again as their doctoral studies, research, and applications proceed.There is moderately good attention paid to pedagogics, but the examples, problems, etc. are far better in reality than a text designed for teaching alone-- they take a "research-reality" approach and give many practical aspects of solutions, including bootstrap methods and shortcuts that get you there but certainly aren't the simpler "mathematical rigor" examples other authors choose for their examples to frankly look smart. Many of these examples show the really tough (as in no apparent solution) things we run into daily in molecular structure, which force us to apply messier numerical methods, sieves, brute force and other tricks, as well as much newer algorithms.The really cool thing about the whole relatively recent (10 years) trend of applying QM an QF techniques to both structure and function problems in molecular and physical chem are the many new tools now available since the particle guys get so many grants!!! These include path integrals, looking at structural elements as operators, not just geometry, new energy and state/structure calcs, perturbation techniques, new statistical methods, and much more.The text/reference is VERY up to date with code, modeling sims, programs, the most recent "named" algorithms, etc. as well as detailed equation applications and examples, INCLUDING Octave/MatLab- ready sequences you can apply more widely (not that 1,000 pages of densely

packed formulas is not broad enough!).An interesting aside is that, unlike a pure "text," there also is original research and equation applications not found either in citations, journals or other texts yet. You can search these on all the databases and pubs-- the authors pull back the curtain on techniques that are state of the art right now, and being practically used in research where intermediate results are too busy to publish every detail vs. the bigger picture.Highly recommended both to extend your toolkit, as an outstanding reference, and as a grad text. If you're undergrad (Senior), it is worth the investment if you are going on to specialize in this application, but I doubt there will be many undergrad classes (maybe an AP lab or seminar?) given on these advanced topics. The professor herself/himself would probably rather keep it!!! I've also error checked with about 60% sampling, and the math is very tight and error free. Authors assume working knowledge of some notation you'd probably explain more thoroughly to undergrads but not grads, like sudden jumps from functions to polynomial generation without the "why", switches in notation between integral and matrix, assumed knowledge of QM constants (more explanation given of QFT constants), a LOT of exponential/ log and trig notation, and of course assumption of previous work with Lagrangians, Laplacians, Gaussians, Fouriers, Monte Carlo, oscillators, Yang-Mills and other gauges, etc.Library Picks reviews only for the benefit of shoppers and has nothing to do with , the authors, manufacturers or publishers of the items we review. We always buy the items we review for the sake of objectivity, and although we search for gems, are not shy about trashing an item if it's a waste of time or money for shoppers. If the reviewer identifies herself, her job or her field, it is only as a point of reference to help you gauge the background and any biases.

Good reference for quantum chemists.

I am so glad to find out this new edition for less than 100 bucks! This is the Bible of quantum chemistry! It covers all the important aspects of wave function theory calculations including practical aspect such as convergence algorithms and integral algorithms. The only thing I wish it covers more is the multi-reference CC and MRCI and DFT, but apart from that, this this the book you are looking for. You may not need this if you are a master degree seeking student, but if you are a phd student working on electronic structure calculation, look no further. If you are a faculty, I'll be surprised if you don't have this book already!

This is one of the greatest scientific monographs ever written. If you are not interested in the material, that's your business, but if you are a quantum chemist or trying to become one, this is the

book you must read. This book covers all of the fundamental material in the field using the modern notation and avoids preserving poor presentations of basic topics which have been kept in other books alive for the sake of history. Each of the authors is a master in his craft and they have spent an extraordinary amount of work to make a book which exceeds all reasonable standards for quality. I won't reiterate the contents of the book since the Table of Contents is quite explicit but it's fair to say each chapter is one of the best presentations of its subject available.The only weakness of this book is that it was meant to be volume one of a two-volume set, but for various reasons, the second volume has never been published. Thus, the authors did not cover their specialty, molecular properties, which is sad given a good book on that topic is missing from the literature. The price is not a weakness because this book is worth every penny of it's list price.If you want less book for less money, these authors have contributed to the ESQC (European Summer School in Quantum Chemistry) Lecture Notes, which can be obtained from (an older version) or from Bjorn Roos at Lund University, for less than half of the cost of this book. Some of the introductory material in this book is reproduced there in an essentially identical form.

This is the Full CI expansion of quantum chemistry literature. High quality, but high price.

Structure and the Properties of Solids: The Physics of the Chemical Bond (Dover Books on Physics) Transition Metal Oxides: An Introduction to Their Electronic Structure and Properties (The International Series of Monographs on Chemistry) Solution Key for Algebra and Trigonometry: Structure and Method: Book 2 (McDougal Littell Structure & Method) Advanced Organic Chemistry: Part A: Structure and Mechanisms: Structure and Mechanisms Pt. A Organic Electronic Materials: Conjugated Polymers and Low Molecular Weight Organic Solids (Springer Series in Materials Science) Molecular Biology: Structure and Dynamics of Genomes and Proteomes Methods in Molecular Biophysics: Structure, Dynamics, Function for Biology and Medicine