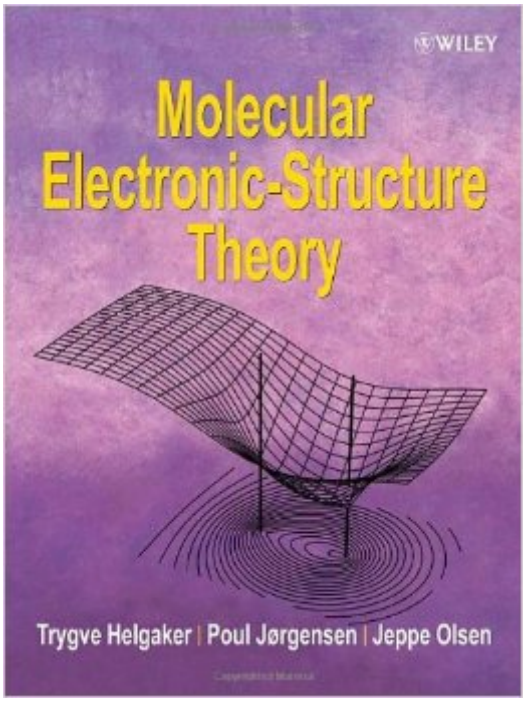
Molecular Electronic-Structure Theory



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.

Book Information

Paperback: 944 pages
Publisher: Wiley; 1 edition (February 18, 2013)
Language: English
ISBN-10: 1118531477
ISBN-13: 978-1118531471
Product Dimensions: 7.5 x 1.9 x 9.7 inches
Shipping Weight: 3.6 pounds (View shipping rates and policies)
Average Customer Review: 5.0 out of 5 starsÂ Â See all reviewsÂ (5 customer reviews)
Best Sellers Rank: #762,381 in Books (See Top 100 in Books) #37 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #59 inÂ Books > Science & Math >

Chemistry > Molecular Chemistry #2034 inÂ Books > Textbooks > Science & Mathematics > Chemistry

Customer Reviews

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.

Phosphodiesterases: Structure, Regulation and Drug Action (Wiley Series in Molecular Pharmacology of Cell Regulation) Biological Inorganic Chemistry, Second Edition: A New Introduction to Molecular Structure and Function Molecular Structure and Dynamics, Volume 16A (Methods in Experimental Physics) Cellular and Molecular Immunology (Cellular and Molecular Immunology, Abbas) Principles of Molecular Virology (Standard Edition), Fourth Edition (Cann, Principles of Molecular Virology) Molecular Pathology of Nervous System Tumors: Biological Stratification and Targeted Therapies (Molecular Pathology Library) High Throughput Screening: Methods and Protocols (Methods in Molecular Biology) (Methods in Molecular Biology, 190) Molecular Visions (Organic, Inorganic, Organometallic) Molecular Model Kit #1 by Darling Models to accompany Organic Chemistry Organic Molecular Photochemistry (Molecular and Supramolecular Photochemistry) Molecular Cell Biology (Lodish, Molecular Cell Biology)