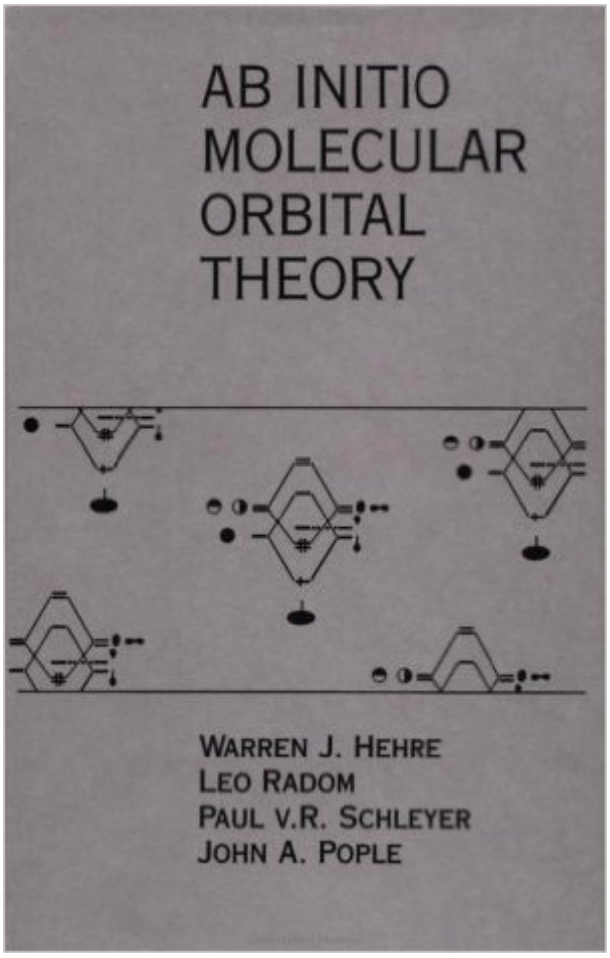
AB INITIO Molecular Orbital Theory



Synopsis

Describes and discusses the use of theoretical models as an alternative to experiment in making accurate predictions of chemical phenomena. Addresses the formulation of theoretical molecular orbital models starting from quantum mechanics, and compares them to experimental results. Draws on a series of models that have already received widespread application and are available for new applications. A new and powerful research tool for the practicing experimental chemist.

Book Information

Hardcover: 576 pages

Publisher: Wiley-Interscience; 1 edition (March 10, 1986)

Language: English

ISBN-10: 0471812412

ISBN-13: 978-0471812418

Product Dimensions: 6.3 x 1.2 x 9.5 inches

Shipping Weight: 2.2 pounds (View shipping rates and policies)

Average Customer Review: 3.7 out of 5 starsÂ Â See all reviewsÂ (3 customer reviews)

Best Sellers Rank: #1,847,451 in Books (See Top 100 in Books) #107 inÂ Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #126 inÂ Books > Science & Math > Chemistry > Molecular Chemistry #1528 inÂ Books > Medical Books > Medicine > Internal Medicine > Pathology > Clinical Chemistry

Customer Reviews

As a graduate student studying quantum chemistry, I find this book useful as a reference. Much of the material is somewhat outdated, but still very applicable and useful for understanding the underlying theory. I would recommend this book for any chemist interested in understanding the theory of quantum chemical calculations or how to interpret the results of such calculations. I would consider it a must for students of quantum, theoretical, or computational chemistry who need to develop an understanding of theory.

This old book attempts to describe basic quantum chemistry and walk one through a series of exercises using the Gaussian series of programs. Not really very useful.

I want of all pictures of orbital structure

AB INITIO Molecular Orbital Theory Life of a Scientist: An Autobiographical Account of the Development of Molecular Orbital Theory Molecular Orbital Studies in Chemical Pharmacology AB INITIO Methods in Quantum Chemistry 2 (Advances in Chemical Physics) (Vol 67) Ab Initio Methods in Quantum Chemistry, Part 1 (Advances in Chemical Physics) The ITU and Managing Satellite Orbital and Spectrum Resources in the 21st Century (SpringerBriefs in Space Development) The Orbital Perspective: Lessons in Seeing the Big Picture from a Journey of 71 Million Miles Orbital Interactions in Chemistry Valency and Bonding: A Natural Bond Orbital Donor-Acceptor Perspective 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) Molecular Red: Theory for the Anthropocene It Does Matter!: Different States of Matter (For Kiddie Learners): Physics for Kids - Molecular Theory (Children's Physics Books) Molecular Symmetry and Group Theory : A Programmed Introduction to Chemical Applications, 2nd Edition Molecular Symmetry and Group Theory