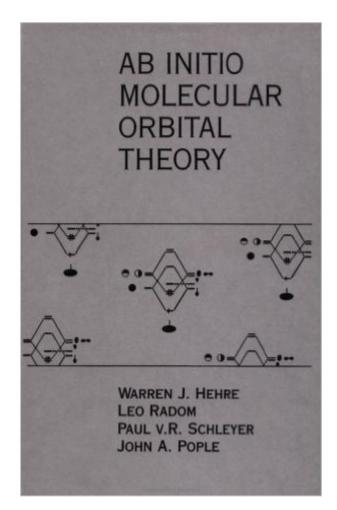
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AB INITIO Molecular Orbital Theory





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 stars Â See all reviews (3 customer reviews) Best Sellers Rank: #1,847,451 in Books (See Top 100 in Books) #107 in Books > Science & Math > Chemistry > Physical & Theoretical > Quantum Chemistry #126 in Books > Science & Math > Chemistry > Molecular Chemistry #1528 in 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 Much of the material is somewhat outdated, but still very applicable and useful for understanding the underlying theory.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.

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