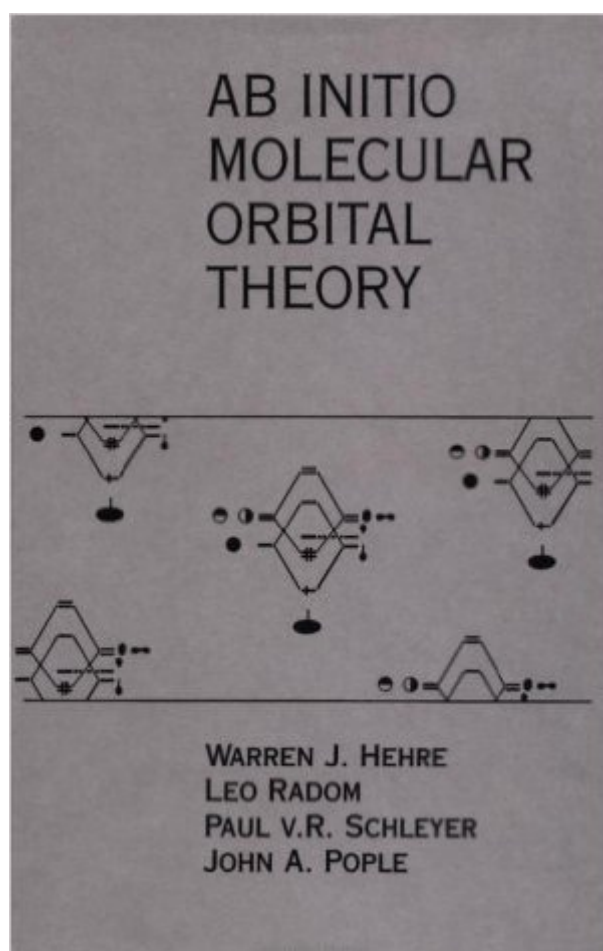


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# AB INITIO Molecular Orbital Theory



## 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

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

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## 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 Much of the material is somewhat outdated, but still very applicable and useful for understanding the underlying theory.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

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