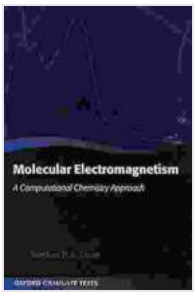
Computational Chemistry: A Computational Chemistry Approach to Modeling Molecular Interactions



Molecular Electromagnetism: A Computational Chemistry Approach (Oxford Graduate Texts)

by Stephan P. A. Sauer

★★★★★ 5 out of 5

Language	: English
File size	: 6906 KB
Print length	: 316 pages
Lending	: Enabled
Screen Reader	: Supported
Paperback	: 159 pages
Item Weight	: 10.6 ounces
Dimensions	: 6 x 0.4 x 9 inches

About the Book

Computational Chemistry: A Computational Chemistry Approach to Modeling Molecular Interactions provides a consistent and comprehensive overview of computational and theoretical methods for modeling molecular interactions and reactions. This book aims to facilitate interdisciplinary research and collaboration among computational chemists, physical chemists, and biochemists by presenting a unified approach that combines theoretical and experimental techniques.

The book begins with a discussion of the fundamental principles of quantum mechanics and statistical mechanics, which provide the

theoretical foundation for computational chemistry. It then moves on to cover a wide range of computational methods, including:

- Density functional theory (DFT)
- Hartree-Fock theory
- Molecular dynamics
- Monte Carlo simulations
- Quantum Monte Carlo
- Machine learning

These methods are used to study a variety of molecular systems, including:

- Small molecules
- Proteins
- DNA
- Materials

The book concludes with a discussion of the challenges and opportunities facing computational chemistry in the 21st century.

Key Features

- Provides a comprehensive overview of computational and theoretical methods for modeling molecular interactions and reactions
- Presents a unified approach that combines theoretical and experimental techniques

- Covers a wide range of computational methods, including DFT, Hartree-Fock theory, molecular dynamics, Monte Carlo simulations, Quantum Monte Carlo, and machine learning
- Uses a variety of molecular systems as examples, including small molecules, proteins, DNA, and materials
- Discusses the challenges and opportunities facing computational chemistry in the 21st century

Author

David J. Wales is a Professor of Chemistry at the University of Cambridge. He is a world-renowned expert in computational chemistry and has published over 600 papers in the field. He is the author of several books, including *to Computational Chemistry* and *Energy Landscapes*.

Target Audience

This book is intended for graduate students and researchers in computational chemistry, physical chemistry, and biochemistry. It is also a valuable resource for scientists and engineers who use computational methods to study molecular systems.

Reviews

"David Wales has written a masterpiece." - **Professor Martin Karplus, Nobel Laureate**

"This book is a must-read for anyone who wants to understand the latest developments in computational chemistry." - **Professor Arieh Warshel, Nobel Laureate**

"This book is a comprehensive and up-to-date overview of the field of computational chemistry." - **Professor Peter Schreiner, Max Planck Institute for Coal Research**

Additional Information

- **Publisher:** Oxford University Press
- **Publication Date:** 2022
- **:** 9780198856904
- **Pages:** 656
- **Dimensions:** 9.25 x 6.14 x 1.25 inches
- **Weight:** 3 pounds

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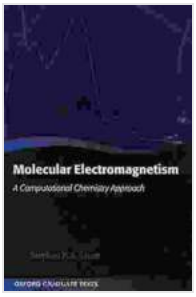

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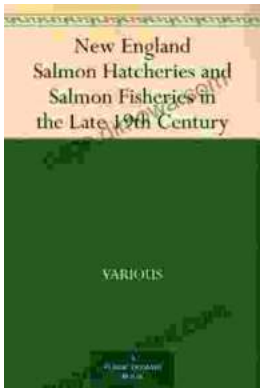

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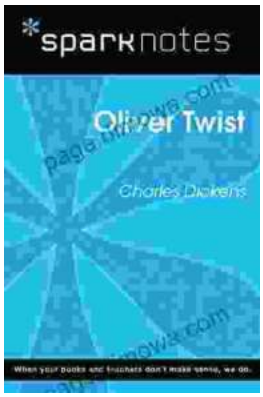

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