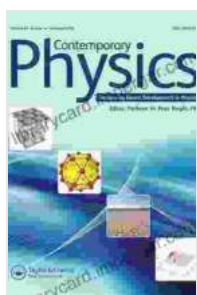


Electronic Structure: Basic Theory and Practical Methods

Embark on a captivating journey into the realm of electronic structure, the cornerstone of modern chemistry and materials science. This comprehensive guide delves into the fundamental principles and practical methods that unlock the secrets of atomic and molecular systems.



Electronic Structure: Basic Theory and Practical Methods by Richard M. Martin

★★★★☆ 4.2 out of 5

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File size : 21762 KB
Text-to-Speech : Enabled
Screen Reader : Supported
Enhanced typesetting : Enabled
Print length : 652 pages

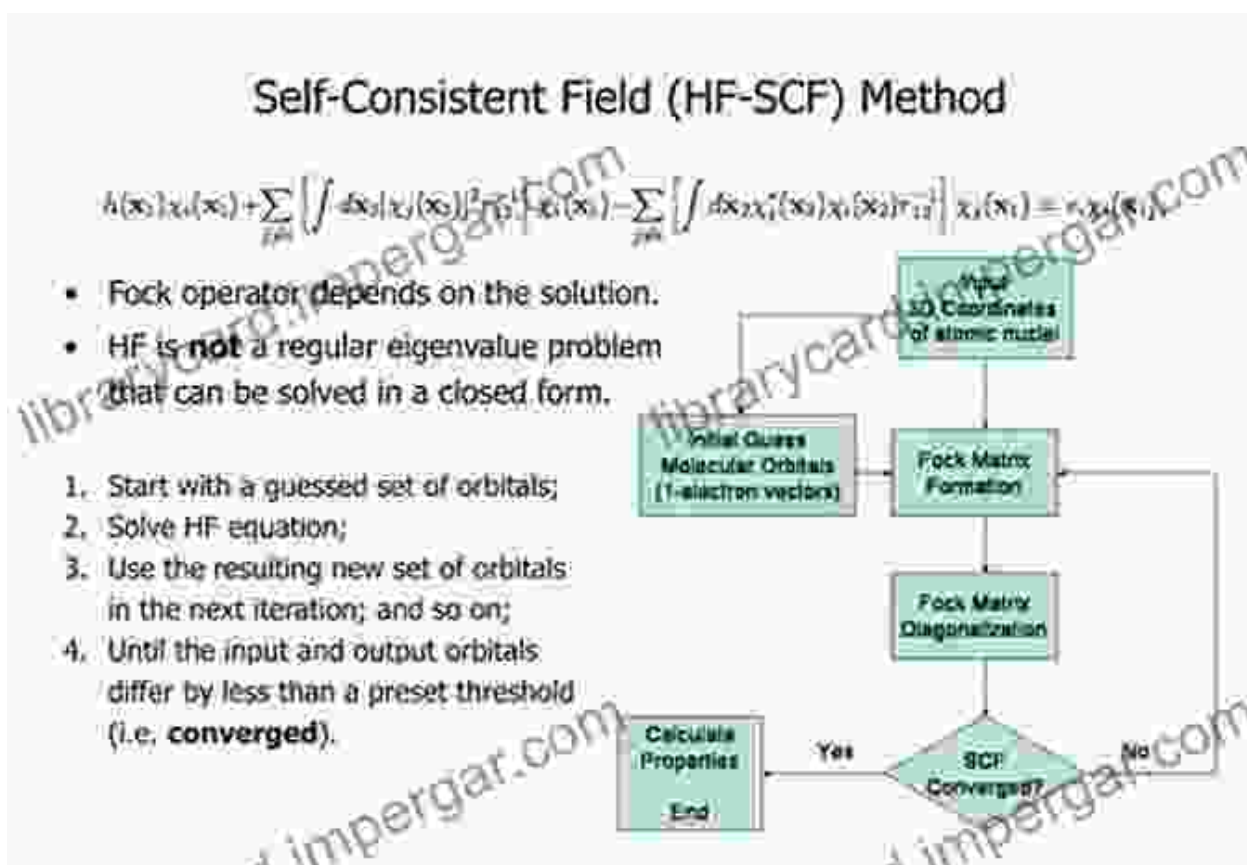


Chapter 1: Fundamental Concepts

Lay the foundation for your understanding of electronic structure with a thorough exploration of:

- The Schrödinger equation: The cornerstone of quantum mechanics
- The variational principle: A powerful tool for approximating solutions
- Molecular orbitals: The building blocks of chemical bonding

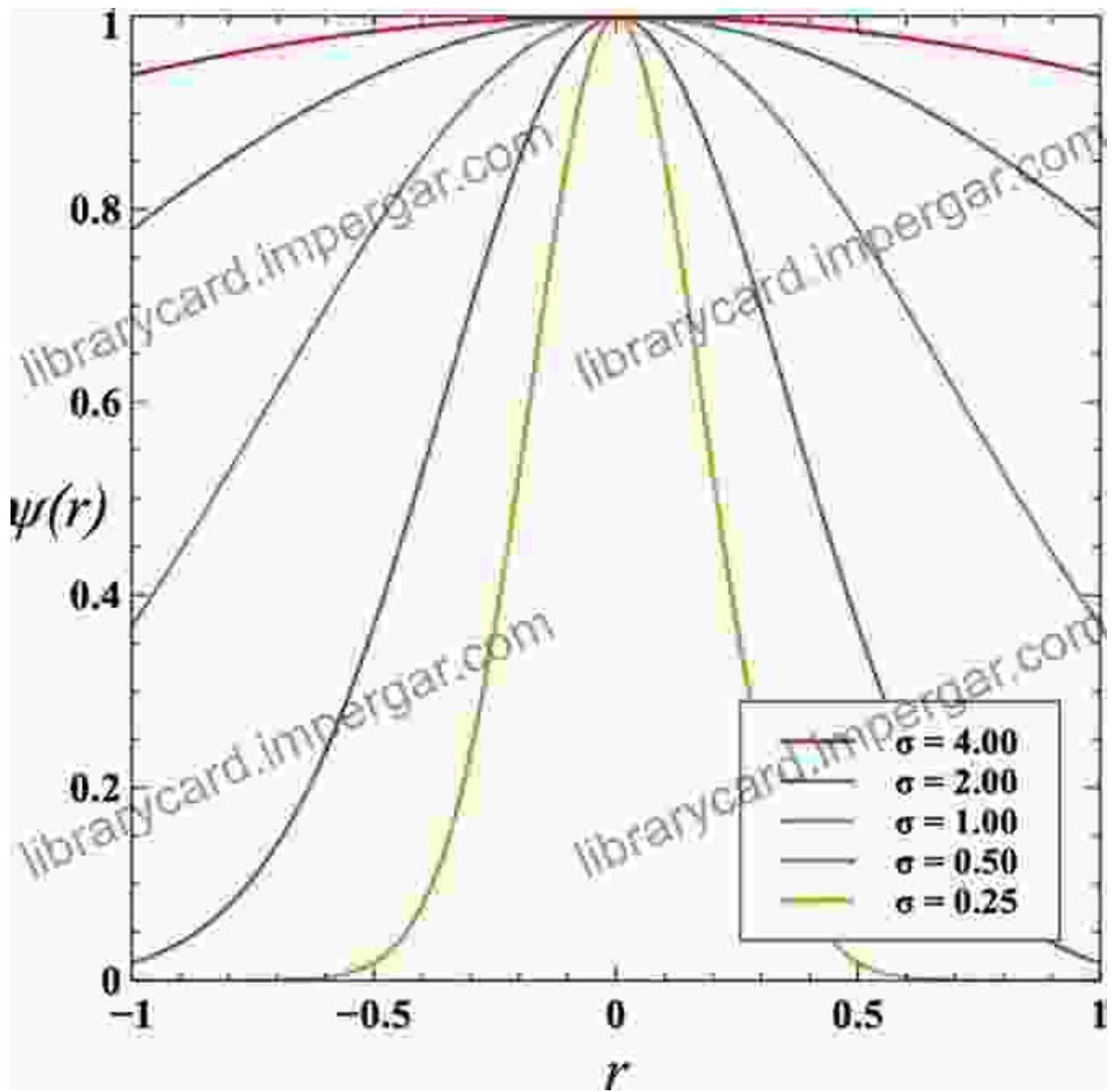
- Density functional theory (DFT): A state-of-the-art method for studying complex systems



Chapter 2: Computational Methods

Delve into the practical aspects of electronic structure calculations with in-depth coverage of:

- Ab initio methods: Calculating energies and properties from first principles
- Semi-empirical methods: Combining experimental data with theoretical approximations



- Numerical methods: Solving the Schrödinger equation on a computer

Chapter 3: Applications in Chemistry and Materials Science

Uncover the practical applications of electronic structure theory in diverse fields, including:

- Quantum chemistry: Understanding chemical bonding and reactivity

- Materials science: Designing new materials with tailored properties
- Biochemistry: Studying the structure and function of biological molecules
- Solid-state physics: Exploring the electronic properties of solids
- Spectroscopy: Identifying and characterizing molecules and materials

Chapter 4: Advanced Topics

Expand your knowledge with in-depth discussions of emerging and advanced concepts, such as:

- Excited states: Exploring electronic transitions and optical properties

Time-Dependent Perturbation Theory (cont.)

Adding Franck-Condon overlap for vibrational wave functions (assuming little interaction with high frequency field)

$$c_{m,n}(t) = \frac{1}{i\hbar} \left[\frac{e^{i(\omega_0 - \omega)t} - 1}{\omega_0 - \omega} \langle \psi_m | \hat{V} | \psi_n \rangle \langle \chi_m | \chi_n \rangle + \frac{e^{i(\omega_0 + \omega)t} - 1}{\omega_0 + \omega} \langle \psi_m | \hat{V} | \psi_n \rangle \langle \chi_m | \chi_n \rangle \right]$$

$\omega = 2\pi\nu$ $\omega_0 = \frac{E_0 - E_1}{\hbar}$

Qualitative points:

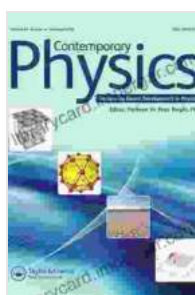
- The second term in brackets becomes large (but remains well behaved based on series expansion of the exponential) when the radiation frequency comes into resonance with the state energy separation
- The transition dipole moment expectation value differentiates the absorption probability of one state from another
- Excited vibrational states should have turning points at the ground-state equilibrium geometry for significant overlap

- Quantum Monte Carlo: A stochastic approach to electronic structure calculations

- Coupled-cluster theory: A highly accurate method for studying small molecules

This comprehensive guide is an indispensable resource for students, researchers, and professionals seeking a deep understanding of electronic structure. Whether you are new to the field or an experienced practitioner, this book will provide you with a solid foundation and equip you with the tools to advance your research and applications.

Free Download your copy today and unlock the secrets of the electronic world!



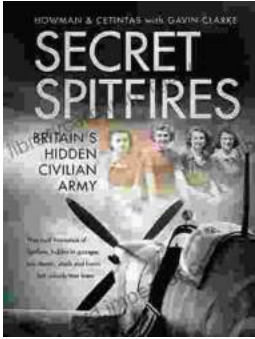
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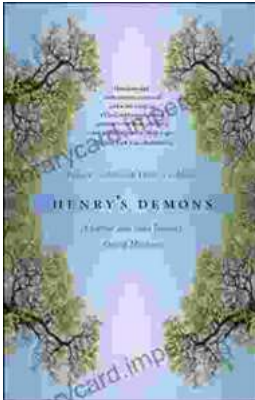
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