



Relativistic Quantum Chemistry: The Fundamental Theory of Molecular Science

Markus Reiher, Alexander Wolf

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Written by two researchers in the field, this book is a reference to explain the principles and fundamentals in a self-contained, complete and consistent way. Much attention is paid to the didactical value, with the chapters interconnected and based on each other. From the contents:

- * Fundamentals
- * Relativistic Theory of a Free Electron: Dirac's Equation
- * Dirac Theory of a Single Electron in a Central Potential
- * Many-Electron Theory I: Quantum Electrodynamics
- * Many-Electron Theory II: Dirac-Hartree-Fock Theory
- * Elimination of the Small Component
- * Unitary Transformation Schemes
- * Relativistic Density Functional Theory
- * Physical Observables and Molecular Properties
- * Interpretive Approach to Relativistic Quantum Chemistry

From beginning to end, the authors deduce all the concepts and rules, such that readers are able to understand the fundamentals and principles behind the theory. Essential reading for theoretical chemists and physicists.

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