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Titolo	Relativistic quantum chemistry [[electronic resource]] : the fundamental theory of molecular science // Markus Reiher and Alexander Wolf
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Altri autori (Persone)	WolfAlexander, Dr.
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Soggetti	Quantum chemistry Chemistry Electronic books.
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Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Relativistic Quantum Chemistry; Contents; Preface; 1 Introduction; 1.1 Philosophy of this Book; 1.2 Short Reader's Guide; 1.3 Notational Conventions and Choice of Units; Part I - Fundamentals; 2 Elements of Classical Mechanics and Electrodynamics; 2.1 Elementary Newtonian Mechanics; 2.1.1 Newton's Laws of Motion; 2.1.2 Galilean Transformations; 2.1.2.1 Relativity Principle of Galilei; 2.1.2.2 General Galilean Transformations and Boosts; 2.1.2.3 Galilei Covariance of Newton's Laws; 2.1.2.4 Scalars, Vectors, Tensors in 3-Dimensional Space 2.1.3 Conservation Laws for One Particle in Three Dimensions 2.1.4 Collection of N Particles; 2.2 Lagrangian Formulation; 2.2.1 Generalized Coordinates and Constraints; 2.2.2 Hamiltonian Principle and Euler-Lagrange Equations; 2.2.2.1 Discrete System of Point Particles; 2.2.2.2 Explicit Example: Planar Pendulum; 2.2.2.3 Continuous Systems of Fields; 2.2.3 Symmetries and Conservation Laws; 2.2.3.1 Gauge Transformations of the Lagrangian; 2.2.3.2 Energy and Momentum Conservation; 2.2.3.3 General Space-Time Symmetries; 2.3 Hamiltonian Mechanics; 2.3.1 Hamiltonian Principle and Canonical Equations

2.3.1.1 System of Point Particles2.3.1.2 Continuous System of Fields; 2.3.2 Poisson Brackets and Conservation Laws; 2.3.3 Canonical Transformations; 2.4 Elementary Electrodynamics; 2.4.1 Maxwell's Equations; 2.4.2 Energy and Momentum of the Electromagnetic Field; 2.4.2.1 Energy and Poynting's Theorem; 2.4.2.2 Momentum and Maxwell's Stress Tensor; 2.4.2.3 Angular Momentum; 2.4.3 Plane Electromagnetic Waves in Vacuum; 2.4.4 Potentials and Gauge Symmetry; 2.4.4.1 Lorentz Gauge; 2.4.4.2 Coulomb Gauge; 2.4.4.3 Retarded Potentials; 2.4.5 Survey of Electro- and Magnetostatics; 2.4.5.1 Electrostatics  
2.4.5.2 Magnetostatics2.4.6 One Classical Particle Subject to Electromagnetic Fields; 2.4.7 Interaction of Two Moving Charged Particles; 3 Concepts of Special Relativity; 3.1 Einstein's Relativity Principle and Lorentz Transformations; 3.1.1 Deficiencies of Newtonian Mechanics; 3.1.2 Relativity Principle of Einstein; 3.1.3 Lorentz Transformations; 3.1.3.1 Definition of General Lorentz Transformations; 3.1.3.2 Classification of Lorentz Transformations; 3.1.3.3 Inverse Lorentz Transformation; 3.1.4 Scalars, Vectors, and Tensors in Minkowski Space; 3.1.4.1 Contra- and Covariant Components  
3.1.4.2 Properties of Scalars, Vectors, and Tensors3.2 Kinematical Effects in Special Relativity; 3.2.1 Explicit Form of Special Lorentz Transformations; 3.2.1.1 Lorentz Boost in One Direction; 3.2.1.2 General Lorentz Boost; 3.2.2 Length Contraction, Time Dilation, and Proper Time; 3.2.2.1 Length Contraction; 3.2.2.2 Time Dilation; 3.2.2.3 Proper Time; 3.2.3 Addition of Velocities; 3.2.3.1 Parallel Velocities; 3.2.3.2 General Velocities; 3.3 Relativistic Dynamics; 3.3.1 Elementary Relativistic Dynamics; 3.3.1.1 Trajectories and Relativistic Velocity; 3.3.1.2 Relativistic Momentum and Energy  
3.3.1.3 Energy-Momentum Relation

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#### Sommario/riassunto

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? 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 Transformati

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