

1. Record Nr.	UNINA9910132160003321
Autore	Reiher Markus
Titolo	Relativistic quantum chemistry : the fundamental theory of molecular science / / Markus Reiher and Alexander Wolf
Pubbl/distr/stampa	Weinheim an der Bergstrasse, Germany : , : Wiley-VCH, , 2015 ©2015
ISBN	3-527-66758-X 3-527-66757-1 3-527-66755-5
Edizione	[Second edition.]
Descrizione fisica	1 online resource (765 p.)
Disciplina	541.28
Soggetti	Quantum chemistry Relativistic quantum theory
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Cover; Title Page; Contents; Preface; Preface to the Second Edition; Preface to the First Edition; 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, and Tensors in Three-Dimensional Space 2.1.3 Basic 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 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 Particles 2.3.1.2 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 Lorenz 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 Magnetostatics 2.4.6 One Classical Particle Subject to
 Electromagnetic Fields; 2.4.7 Interaction of Two Moving Charged
 Particles; Further Reading; 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 Transformation
 Properties of Scalars, Vectors, and Tensors; 3.2 Kinematic 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

Sommario/riassunto

Einstein proposed his theory of special relativity in 1905. For a long time it was believed that this theory has no significant impact on chemistry. This view changed in the 1970's when it was realized that (nonrelativistic) Schrodinger quantum mechanics yields results on molecular properties that depart significantly from experimental results. Especially when heavy elements are involved, these quantitative deviations can be so large that qualitative chemical reasoning and understanding is affected. For this to grasp the appropriate many-electron theory has rapidly evolved. Nowadays relativist...
