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Non-covariant Interactions in Quantum Chemistry and Physics-Alberto Otero de la Rua 2017-06-15 Non-covariant Interactions in Quantum Chemistry and Physics: Theory and Applications provides an entry point for newcomers and a standard reference for researchers publishing in the area of non-covariant interactions. Written by the leading experts in this field, the book enables experienced researchers to keep up with the most recent developments in the field. Also, the book provides a comprehensive, in-depth overview of the available quantum-chemistry methods for non-covariant interactions and details the most relevant fields of applications. The text is divided into two parts. The first part contains chapters which allow the reader to grasp the strengths and weaknesses of different computational techniques. Summaries of the state-of-the-art in the computational intermolecular interactions field in a comprehensive work introduces students and researchers from related fields to the basic principles of this field. The second part of the book presents the theoretical foundations of current quantum mechanical methodologies alongside a collection of examples on how they can be applied to solve practical problems.

Recent Advances in Density Functional Methods-Delano P Chong 1997-05-14 Of all the different areas in computational chemistry, density functional theory (DFT) enjoys the most rapid development. Even at the level of the local density approximation (LDA), which is computationally less demanding than DFT, can usually provide better answers than Hartree-Fock formalism for large systems such as clusters and solids. For atoms and molecules, the results from DFT are often superior to those obtained from semi-empirical quantum mechanics methods. The book puts theory and applications side-by-side and allows the reader to grasp the strengths and weaknesses of different techniques. It gives a comprehensive, in-depth overview of the available quantum-chemistry methods for non-covariant interactions and details the most relevant fields of applications. The text is divided into two parts. The first part contains chapters which allow the reader to grasp the strengths and weaknesses of different computational techniques. Summaries of the state-of-the-art in the computational intermolecular interactions field in a comprehensive work introduces students and researchers from related fields to the basic principles of this field. The second part of the book presents the theoretical foundations of current quantum mechanical methodologies alongside a collection of examples on how they can be applied to solve practical problems.

A Primer in Density Functional Theory-Carlson Fischia 2008-01-11 Density functional theory (DFT) is by now a well established approach to theoretical chemistry for the study of the electronic structure of matter. The present book puts theory and applications side-by-side and allows the reader to grasp the strengths and weaknesses of different techniques. It gives a comprehensive, in-depth overview of the available quantum-chemistry methods for non-covariant interactions and details the most relevant fields of applications. The text is divided into two parts. The first part contains chapters which allow the reader to grasp the strengths and weaknesses of different computational techniques. Summaries of the state-of-the-art in the computational intermolecular interactions field in a comprehensive work introduces students and researchers from related fields to the basic principles of this field. The second part of the book presents the theoretical foundations of current quantum mechanical methodologies alongside a collection of examples on how they can be applied to solve practical problems.

Materials Modelling Using Density Functional Theory-Feliciano Giustino 2014-11-20 This book is an introduction to the modern quantum theory of materials, and primarily addresses senior undergraduate and first-year graduate students in chemistry, physics, and materials science and engineering. As advanced materials are becoming ubiquitous in every aspect of our life, the use of quantum mechanics to understand, predict, and control their properties in order to further improve real-world materials and devices is of paramount importance. The modern quantum theory of matter, and in particular density functional theory (DFT) is the bridge that connects atomistic models to macroscopic observations. It is considered one of the most important advances in theoretical physics since the advent of quantum mechanics in the past century. The book is aimed at graduate students and faculty researchers who have a background in physics, mathematics, or chemistry. The book is designed to be self-contained, and it can be used as a reference book or in industry, graduate students.

Electronic Structure Calculations on Graphics Processing Units-Andrews W. Goot 2015-04-26 Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics provides an overview of computing on graphics processing units (GPUs), a brief introduction to GPU programming, and the latest techniques for GPU programming for the most widespread electronic structure methods. The book covers all commonly used basis sets including localized Gaussian and Slater type basis functions, plane waves, wavelets and real-space grid-based approaches. The chapters detail the calculation of electronic states for real materials using state-of-the-art electronic structure methods. The book is primarily intended for advanced students, including PhD students, with a background in condensed matter physics, materials physics, or chemistry. It can be used as a textbook for graduate students and researchers in the field of condensed matter physics, as well as a reference book for researchers in related fields, such as materials science and engineering.

Electronic structure calculations on graphics processing units-Andrews W. Goot 2015-04-26 Electronic Structure Calculations on Graphics Processing Units: From Quantum Chemistry to Condensed Matter Physics provides an overview of computing on graphics processing units (GPUs), a brief introduction to GPU programming, and the latest techniques for GPU programming for the most widespread electronic structure methods. The book covers all commonly used basis sets including localized Gaussian and Slater type basis functions, plane waves, wavelets and real-space grid-based approaches. The chapters detail the calculation of electronic states for real materials using state-of-the-art electronic structure methods. The book is primarily intended for advanced students, including PhD students, with a background in condensed matter physics, materials physics, or chemistry. It can be used as a textbook for graduate students and researchers in the field of condensed matter physics, as well as a reference book for researchers in related fields, such as materials science and engineering.

A Chemist’s Guide to Density Functional Theory-Wolfram Koch 2015-11-18 “Chemists familiar with computational chemistry and physical chemistry, and in materials science and engineering. As advanced materials are becoming ubiquitous in every aspect of our life, the use of quantum mechanics to understand, predict, and control their properties in order to further improve real-world materials and devices is of paramount importance. The modern quantum theory of matter, and in particular density functional theory (DFT) is the bridge that connects atomistic models to macroscopic observations. It is considered one of the most important advances in theoretical physics since the advent of quantum mechanics in the past century. The book is aimed at graduate students and faculty researchers who have a background in physics, mathematics, or chemistry. The book is designed to be self-contained, and it can be used as a reference book or in industry, graduate students.

Computational Electrochemistry-S. Paddison 2015-12-28 Computational Electrochemistry provides a broad introduction to this dynamic subject. Suitable for both experimentalists and theoretical chemists, this book is divided into 15 key areas and covers the latest developments in the field. The book is aimed at advanced students and researchers in the fields of materials science, chemistry, and physics. It provides a comprehensive overview of the computational methods used in electrochemistry, including density functional theory, ab initio quantum chemistry, and classical molecular dynamics. The book also covers the applications of these methods to real-world problems, such as the design of new materials for energy storage and conversion.

Essentials of Computational Chemistry-Joachim Cramer 2013-06-30 Essentials of Computational Chemistry provides a broad introduction to this dynamic subject. Suitable for both experimentalists and theoretical chemists, this book is divided into 15 key areas and covers the latest developments in the field. The book is aimed at advanced students and researchers in the fields of materials science, chemistry, and physics. It provides a comprehensive overview of the computational methods used in electrochemistry, including density functional theory, ab initio quantum chemistry, and classical molecular dynamics. The book also covers the applications of these methods to real-world problems, such as the design of new materials for energy storage and conversion.

Density-Functional Theory of Atoms and Molecules-Robert Parr 1994-05-26密度泛函理论是原子和分子理论的基础，原子和分子物理，密度泛函理论是原子和分子物理理论的基础。密度泛函理论是量子化学中的一个非常重要的分支，它在原子结构、分子结构、分子光谱和分子化学反应等方面都有着广泛的应用。密度泛函理论的出现使得许多以前难以解决的问题变得简单可行，比如分子结构的精确计算、化学反应路径的预测、分子性质的预测等。密度泛函理论的发展也促进了量子化学的其他分支，如量子化学的计算方法和计算的理论基础。密度泛函理论的发展使得量子化学成为了一个非常活跃和重要的领域，它在原子物理学、化学物理学和材料科学研究中都有着广泛的应用。


Molecular Electronic-Structure Theory—B. Yarkony 1995

Modern Electronic Structure Theory—D. R. Yarkony 1995

Tensor network is a fundamental mathematical tool with a wide range of applications in physics, such as condensed matter physics, statistical physics, high energy physics, and condensed-matter physics. Tensor networks provide a natural framework for the representation of quantum states and their entanglement properties. They have been successfully applied to a variety of problems, including quantum many-body systems, quantum information theory, and quantum computing.

The book introduces and reviews recent advances in computational methods for electronic structure calculations, explaining their limitations and advantages and providing examples of their applications. The first part outlines the methods, the second part describes the applications, and the third part discusses the future of the field.


The book covers a broad range of topics, including the theoretical foundations of computational chemistry, various methods for calculating molecular properties, and applications of these methods to real-world problems. It is intended for graduate students, researchers, and practitioners in the field of computational chemistry.

Tensor network conceptions—Sho-Ran 2020

Tensor network is a fundamental mathematical tool that plays a central role in modern physics. It is used to describe and analyze quantum systems, including quantum many-body systems, quantum entanglement, quantum computation, and quantum information theory. Tensor networks provide a powerful framework for understanding and exploiting the behavior of quantum systems, and they have applications in a wide range of fields, including condensed matter physics, statistical mechanics, and quantum chemistry.

Tensor network methods are particularly useful for studying quantum systems with long-range correlations, such as quantum critical points, quantum phase transitions, and quantum spin liquids. They allow for the efficient and accurate calculation of ground states and excited states of quantum systems, and they can be applied to both small and large systems.

The book provides a comprehensive introduction to tensor networks, covering both the theoretical foundations and practical applications. It includes detailed discussions of various tensor network algorithms, such as matrix-product states, cluster-state methods, and projected entangled pair states. The book also discusses the interplay between tensor networks and other quantum information processing techniques, such as quantum error correction and quantum algorithms.
The book aims to provide a detailed introduction to the state-of-the-art covariant density functional theory, which follows the Lorentz invariance from the very beginning and is able to describe nuclear many-body quantum systems microscopically and self-consistently. Covariant density functional theory was introduced in nuclear physics in the 1970s and has since been developed and used to describe the diversity of nuclear properties and phenomena with great success. In order to provide an advanced and updated textbook of covariant density functional theory for graduate students and nuclear physics researchers, this book summarizes the enormous amount of material that has accumulated in the field of covariant density functional theory over the last few decades as well as the latest developments in this area. Moreover, the book contains enough details for readers to follow the formalism and theoretical results, and provides exhaustive references to explore the research literature.

Contents:
- Concept of Covariant Density Functional Theory
- Relativistic Mean-Field Description of Nuclei
- Relativistic Hartree-Fock-Bogoliubov Theory
- Nuclear Shell Structure and Response
- Beyond Mean-Field Approximation
- Heavy Element in Astrophysical Nucleosynthesis
- Computational Chemistry: Reviews of Current Trends, Vol. 1
- Computational Chemistry: Reviews of Current Trends, Vol. 2
- Computational Chemistry: Reviews of Current Trends, Vol. 3

The authors include all the experts in this field including many world-leading scientists from China, Europe, Japan, and the United States. Keywords: Covariant Density Functional Theory, Relativistic Mean-Field, Pairing Correlations, Exotic Nuclei, Hypernuclei, Well-Deformed and Superdeformed Nuclei, Pairing, Transition, Rotation, Collective Excitations, Small Amplitude Motion, Quadrupole-Vibration Coupling, Beyond Mean-Field Approximation, Astrophysical Nucleosynthesis, Neutron Star

Computational Chemistry: Reviews Of Current Trends, Vol. 1-Nicholas Bodor 1996-02-16 This book presents an overview of recent progress in computational techniques as well as examples of the application of existing computational methods in different areas of chemistry, physics, and biochemistry. Introductory chapters cover a broad range of fundamental topics, including: state-of-the-art basin set expansion methods for computing atomic and molecular electronic structures based on the use of relativistic quantum mechanics; the most recent developments in Hartree-Fock methods, particularly in techniques suited for very large systems; the current analysis of the solvatochromic free-energy of interaction and the physical bases used to evaluate the electrostatic, cavitation, and dispersion terms; an introduction to the additive fuzzy electron density fragmentation scheme within various ab initio Hartree-Fock quantum-chemical computational schemes, which has provided the means for generating representative molecular fragment densities characteristic to their local environment within a molecule. This book also features a review of recent ab initio calculations on the structure and interactions of DNA bases, a chapter on computational approaches to the design of safer drugs and their molecular properties, and a systematic conceptual study on a route which allows one to stuff fullerenes.

Concepts and Methods in Modern Theoretical Chemistry-Swapan Kumar Ghosh 2016-04-19 Concepts and Methods in Modern Theoretical Chemistry: Electronic Structure and Reactivity, the first book in a two-volume set, focuses on the structure and reactivity of systems and phenomena. A new addition to the series Atoms, Molecules, and Clusters, this book offers chapters written by experts in their fields. It enables readers to learn how concepts from ab initio quantum chemistry and density functional theory (DFT) can be used to describe, understand, and predict electronic structure and chemical reactivity. This book covers a wide range of subjects, including discussions on the following topics: DFT, particularly the functional and conceptual aspects Excluded states, molecular electronic potentials, and intermolecular interactions General theoretical aspects and application to molecules Clusters and solids, electronic stress, and electron affinity difference The information theory and the virial theorem New periodic tables The role of the ionization potential Although most of the chapters are written at a level that is accessible to a senior graduate student, experienced researchers will also find interesting new insights in these experts’ perspectives. This comprehensive book provides an invaluable resource toward understanding the whole gamut of atoms, molecules, and clusters.