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Descrizione fisica	1 online resource (410 p.)
Collana	Mathematical Physics Studies, , 0921-3767
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Soggetti	Mathematical physics Chemistry, Physical and theoretical Artificial intelligence Theoretical, Mathematical and Computational Physics Theoretical and Computational Chemistry Mathematical Physics Artificial Intelligence
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references at the end of each chapters.
Nota di contenuto	Topics in Quantum Chemistry -- Relativistic Quantum Theory of Many-Electron Systems -- Spurious Modes in Dirac Calculations and how to avoid them -- Tensor product approximation (DMRG) and Coupled Cluster Method in Quantum Chemistry -- Quantum Cluster Equilibrium -- Linear Response Methods in Quantum Chemistry -- Topics in Density Functional Theory and Related Approaches -- Progress on New Approaches to Old Ideas: Orbital-free Density Functionals -- Time-dependent Density Functional Theory -- Density Functional Theory for Strongly-Interacting Electrons -- Towards the Computational Design of Compounds from First Principles -- Application of (Kohn-Sham) Density Functional Theory to Real Materials -- The Quantum Energy agrees with the M•uller Energy up to the Third Order -- Mathematical Aspects of Density Functionals and Density Matrix Functionals in Quantum Chemistry -- Some (important?) unsolved Mathematical Problems in Molecular Simulation -- Topics in Computer Science -- The Computational Complexity of Density Functional Theory --

Computational Techniques for Density Functional-based Molecular Dynamics Calculations in Plane-Wave and Localized Basis Sets -- Information Theory in Many-Electron Descriptions -- Towards the Information-Theoretic Construction of an Orbital-free Kinetic Energy Functional -- Lieb-Robinson Bounds and Simulation of Time Evolution of Local Observables in Lattice Systems -- Green Function-based Approaches -- Electronic Structure Calculations with LDA+DMFT -- The GW Approximation for the Electronic Self-Energy -- Topics in Quantum Monte Carlo and Related Approaches -- Levy-Lieb Principle meets Quantum Monte Carlo -- The new Resonating Valence Bond Method for ab-initio Electronic Simulations. Mathematical Perspective on Quantum Monte Carlo Methods -- Open Problems: A wish list of Mel Levy and Elliot Lieb.

Sommario/riassunto

This book provides a broad description of the development and (computational) application of many-electron approaches from a multidisciplinary perspective. In the context of studying many-electron systems Computer Science, Chemistry, Mathematics and Physics are all intimately interconnected. However, beyond a handful of communities working at the interface between these disciplines, there is still a marked separation of subjects. This book seeks to offer a common platform for possible exchanges between the various fields and to introduce the reader to perspectives for potential further developments across the disciplines. The rapid advances of modern technology will inevitably require substantial improvements in the approaches currently used, which will in turn make exchanges between disciplines indispensable. In essence this book is one of the very first attempts at an interdisciplinary approach to the many-electron problem.