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Titolo	Strategies and applications in quantum chemistry [[electronic resource]] : from molecular astrophysics to molecular engineering / / edited by Y. Ellinger and M. Defranceschi
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Collana	Topics in molecular organization and engineering ; ; v. 14
Altri autori (Persone)	EllingerY DefranceschiMireille <1955->
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Soggetti	Quantum chemistry Electronic books.
Lingua di pubblicazione	Inglese
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Note generali	Description based upon print version of record.
Nota di bibliografia	Includes bibliographical references and index.
Nota di contenuto	Quantum Chemistry: The New Frontiers -- Quantum Chemistry: The New Frontiers -- Strategies and Formalisms -- Theory of Orbital Optimisation in SCF and MCSCF Calculations -- A Coupled MCSCF-perturbation Treatment for Electronic Spectra -- Reduced Density Matrix versus Wave Function: Recent Developments -- The Real Generators of the Unitary Group -- Convergence of Expansions in a Gaussian Basis -- Quantum Chemistry in Front of Symmetry-breakings -- Molecular Orbital Electronegativity as Electron Chemical Potential in Semiempirical SCF Schemes -- Quasicrystals and Momentum Space -- Quantum Chemistry Computations in Momentum Space -- Core-valence Separation in the Study of Atomic Clusters -- Core-hole States and the Koopmans Theorem -- An Application of the Half-projected Hartree-Fock Model to the Direct Determination of the Lowest Singlet and Triplet Excited States of Molecular Systems -- FSGO Hartree-Fock Instabilities of Hydrogen in External Electric Fields -- Electronic Charge Density of Quantum Systems in the Presence of an Electric Field: a Search for Alternative Approaches -- How Much Correlation Can We Expect to Account for in Density Functional Calculations ? Case Studies

of Electrostatic Properties of Small Molecules -- Applications of Nested Summation Symbols to Quantum Chemistry: Formalism and Programming Techniques -- Applications to Physical Phenomena -- Vibrational Modulation Effects on EPR Spectra -- Ab-initio Calculations of Polarizabilities in Molecules: Some Proposals to this Challenging Problem -- Coupled Hartree-Fock Approach to Electric Hyperpolarizability Tensors in Benzene -- Second Order Static Hyperpolarizabilities of Insaturated Polymers -- An ab initio Study of the Magnetic Properties of the Isoelectronic Series BeH?, BH, CH+ and MgH?, AlH, SiH+ -- CI Calculations of Miscellaneous Spectroscopic Observables for the PN X1?, A1? and 1? States -- Theoretical Treatment of State-selective Charge Transfer Processes. N5++He as a Case Study -- An Ab initio Study of the Lowest 1,3?+ States of BH. Quasi Diabatic Curves and Vibronic Couplings -- Magnesium Photoionization: a K-matrix Calculation with GTO Bases -- Investigation of Photochemical Paths by a Combined Theoretical and Experimental Approach -- C3H2: A Puzzling Interstellar Small Molecule -- Ab-initio Study of the Intramolecular Hydrogen Shift in Nitromethane and its Acid-dissociated Anion -- From Cluster to Infinite Solid: a Quantum Study of the Electronic Properties of MoO3 -- Ab initio Calculations on Muonium Adducts of Fullerenes.

Sommario/riassunto

At the time when increasing numbers of chemists are being attracted by the fascination of supposedly easy computing and associated colourful imaging, this book appears as a counterpoint. The first part focuses on fundamental concepts of quantum chemistry, covering MCSCF theory, perturbation treatments, basis set developments, density matrices, wave function instabilities to correlation effects, and momentum space theory. The second part is devoted to more practical studies, ranging from the characterisation of exotic interstellar molecules, the accurate determination of spectroscopic constants, excited states structures and EPR parameters through photochemical and charge-transfer processes, cluster chemistry and fullerenes, muonium chemistry, to the possible prediction of the response of materials to electric fields in view of nonlinear optical applications. Audience: Graduate students and researchers whose work involves quantum chemistry, molecular physics, and materials modelling.