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Disciplina	541.2
Soggetti	Chemistry, Physical and theoretical Chemistry - Data processing Atoms Molecules Quantum theory Molecules - Models Theoretical Chemistry Computational Chemistry Atomic, Molecular and Chemical Physics Quantum Physics Physical Chemistry Molecular Modelling
Lingua di pubblicazione	Inglese
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Nota di contenuto	Introduction -- General Definitions -- Time-Independent Electron Current Density -- Time-Dependent Perturbations -- Implementation of Origin-Independent Dynamic Polarizability Density Within Coupled Cluster Response Theory -- Conclusions and Outlook.
Sommario/riassunto	This book outlines past and new developments in molecular response theory in terms of static and dynamic-induced current densities and showcases an important step forward in the field of molecular density functions and their topological analysis. The book begins with a general perspective on topics such as classical Hamiltonian, quantum

mechanical Hamiltonian, and topological analysis of the electron charge density, followed by an in-depth overview of time-dependent and -independent perturbations, and applications. In this book, the author presents a completely new approach that allows the interpretation of electric and magnetic properties through origin-independent density functions. Readers will also find examples of how the new origin-independent density functions are useful for rationalizing the chemical behavior of molecules interacting with impinging radiation. The concepts contained within the book are the basis for a deeper understanding of Nuclear magnetic resonance (NMR) and Electron paramagnetic resonance (EPR) spectroscopies, as well as the mechanisms that give rise to electric polarization and optical activity in chiral systems. A basic knowledge of quantum mechanics and ab initio electronic structure calculation methods such as Hartree-Fock and Density Functional Theory is required. Given its breadth, the book provides an important contribution to the field of Quantum Chemical Topology and appeals to students and researchers interested in learning more about the relationship between electrical and magnetic properties, density functions derivable from them and experimental observables.
