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Disciplina	541.39
Soggetti	Chemistry, Physical and theoretical Chemistry, Inorganic Theoretical and Computational Chemistry Physical Chemistry Inorganic Chemistry
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Nota di contenuto	From the phenomenology of chemical reactions to the study of two body collisions -- A quantum approach to the two body problem -- Ab initio electronic structure for few body systems -- The treatment of few body reactions -- Complex reactive applications: a forward look to Open Science -- Appendices.
Sommario/riassunto	This graduate textbook, written by experienced lecturers, features the study and computation of efficient reactive processes.The text begins with the problem of determining the chemical reaction properties by first decomposing complex processes into their elementary components. Next, the problem of two colliding mass points is investigated and relationships between initial conditions and collision outcomes are discussed. The failure of classical approaches to match experimental information is discussed and a quantum formulation of the calculation of the properties of two colliding bodies is provided. The authors go onto describe how the formalism is extended to structured collision partners by discussing the methods used to compute the electronic structure of polyelectronic reactants and products and the formalism of atom diatom reactions. Additionally, the

relationships between the features of the potential energy surface and the outcomes of the reactive dynamics, are discussed. Methods for computing quantum, classical, and semi-classical reactive probabilities based on the already discussed concepts and tools are also featured and the resulting main typical reactive behaviors are analyzed. Finally, the possibility of composing the computational tools and technologies needed to tackle more complex simulations as well as the various competences and distributed computing infrastructure needed for developing synergistic approaches to innovation are presented.