1. Record Nr. UNINA9910457732603321 Autore Levine Raphael D. Titolo Molecular reaction dynamics / / Raphael Levine [[electronic resource]] Cambridge:,: Cambridge University Press,, 2005 Pubbl/distr/stampa **ISBN** 1-107-14046-3 1-282-39414-2 9786612394140 0-511-64365-9 0-511-19639-3 0-511-08081-6 0-511-56749-9 0-511-61412-8 0-511-08005-0 1 online resource (xiv, 554 pages) : digital, PDF file(s) Descrizione fisica 541/.394 Disciplina Soggetti Molecular dynamics Chemical reaction, Conditions and laws of Lingua di pubblicazione Inglese **Formato** Materiale a stampa Livello bibliografico Monografia Note generali Title from publisher's bibliographic system (viewed on 05 Oct 2015). Nota di bibliografia Includes bibliographical references (p. 500-541) and index. Nota di contenuto 1. Understanding chemical reactions at the molecular level: 2. Molecular collisions; 3. Introduction to reactive molecular collisions; 4. Scattering as a probe of collision dynamics; 5. Introduction to polyatomic dynamics; 6. Structural considerations in the calculation of reaction rates; 7. Photoselective chemistry: access to the transition state region; 8. Chemistry in real time; 9. State-changing collisions: molecular energy transfer; 10. Stereodynamics; 11. Dynamics in the condensed phase; 12. Dynamics of gas-surface interactions and reactions; Bibliography; Index. Sommario/riassunto Molecular reaction dynamics is the study of chemical and physical transformations of matter at the molecular level. The understanding of how chemical reactions occur and how to control them is fundamental to chemists and interdisciplinary areas such as materials and

nanoscience, rational drug design, environmental and astrochemistry.

This book provides a thorough foundation to this area. The first half is introductory, detailing experimental techniques for initiating and probing reaction dynamics and the essential insights that have been gained. The second part explores key areas including photoselective chemistry, stereochemistry, chemical reactions in real time and chemical reaction dynamics in solutions and interfaces. Typical of the new challenges are molecular machines, enzyme action and molecular control. With problem sets included, this book is suitable for advanced undergraduate and graduate students, as well as being supplementary to chemical kinetics, physical chemistry, biophysics and materials science courses, and as a primer for practising scientists.