

1. Record Nr.	UNINA9910254147103321
Autore	Gatti Fabien
Titolo	Applications of Quantum Dynamics in Chemistry // by Fabien Gatti, Benjamin Lasorne, Hans-Dieter Meyer, André Nauts
Pubbl/distr/stampa	Cham : , : Springer International Publishing : , : Imprint : Springer, , 2017
ISBN	3-319-53923-X
Edizione	[1st ed. 2017.]
Descrizione fisica	1 online resource (XVI, 429 p. 110 illus.)
Collana	Lecture Notes in Chemistry, , 0342-4901 ; ; 98
Disciplina	541.28
Soggetti	Chemistry, Physical and theoretical Quantum theory Cheminformatics Chemometrics Theoretical and Computational Chemistry Quantum Physics Computer Applications in Chemistry Math. Applications in Chemistry
Lingua di pubblicazione	Inglese
Formato	Materiale a stampa
Livello bibliografico	Monografia
Nota di bibliografia	Includes bibliographical references at the end of each chapters and index.
Nota di contenuto	Part I Introduction -- Part II Concepts and Methods: Quantum effects -- Electronic states and potential energy operators -- The Choice of coordinates -- Kinetic energy operators -- Introduction to molecular symmetry -- Introduction to numerical methods and to MCTDH -- Part III Applications: Infrared spectroscopy -- Quantum control with laser pulses in the electronic ground state -- Photodissociation spectra -- Cross sections for reactive scattering -- Quantum control with laser pulses for electronically excited states -- Non-adiabatic photochemistry -- Optimal control and quantum computers -- Part IV Conclusion.
Sommario/riassunto	This book explains the usage and application of Molecular Quantum Dynamics, the methodology where both the electrons and the nuclei in a molecule are treated with quantum mechanical calculations. This volume of Lecture Notes in Chemistry addresses graduate students and

postdocs in the field of theoretical chemistry, as well as postgraduate students, researchers and teachers from neighboring fields, such as quantum physics, biochemistry, biophysics, or anyone else who is interested in this rising method in theoretical chemistry, and who wants to gain experience in the opportunities it can offer. It can also be useful for teachers interested in illustrative examples of time-dependent quantum mechanics as animations of realistic wave packets have been designed to assist in visualization. Assuming a basic knowledge about quantum mechanics, the authors link their explanations to recent experimental investigations where Molecular Quantum Dynamics proved successful and necessary for the understanding of the experimental results. Examples including reactive scattering, photochemistry, tunneling, femto- and attosecond chemistry and spectroscopy, cold chemistry or crossed-beam experiments illustrate the power of the method. The book restricts complicated formalism to the necessary and in a self-contained and clearly explained way, offering the reader an introduction to, and instructions for, practical exercises. Continuitive explanation and math are optionally supplemented for the interested reader. The reader learns how to apply example simulations with the MCTDH program package (Multi Configuration Time Dependent Hartree calculations). Readers can thus obtain the tools to run their own simulations and apply them to their problems. Selected scripts and program code from the examples are made available as supplementary material. This book bridges the gap between the existing textbooks on fundamental theoretical chemistry and research monographs focusing on sophisticated applications. It is a must-read for everyone who wants to gain a sound understanding of Molecular Quantum Dynamics simulations and to obtain basic experience in running their own simulations.
