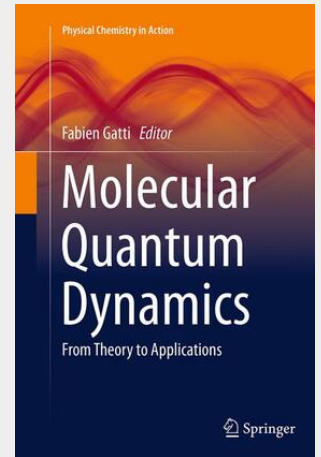


Gatti

Molecular Quantum Dynamics

From Theory to Applications

This book focuses on current applications of molecular quantum dynamics. Examples from all main subjects in the field, presented by the internationally renowned experts, illustrate the importance of the domain. Recent success in helping to understand experimental observations in fields like heterogeneous catalysis, photochemistry, reactive scattering, optical spectroscopy, or femto- and attosecond chemistry and spectroscopy underline that nuclear quantum mechanical effects affect many areas of chemical and physical research. In contrast to standard quantum chemistry calculations, where the nuclei are treated classically, molecular quantum dynamics can cover quantum mechanical effects in their motion. Many examples, ranging from fundamental to applied problems, are known today that are impacted by nuclear quantum mechanical effects, including phenomena like tunneling, zero point energy effects, or non-adiabatic transitions. Being important to correctly understand many observations in chemical, organic and biological systems, or for the understanding of molecular spectroscopy, the range of applications covered in this book comprises broad areas of science: from astrophysics and the physics and chemistry of the atmosphere, over elementary processes in chemistry, to biological processes (such as the first steps of photosynthesis or vision). Nevertheless, many researchers refrain from entering this domain. The book "Molecular Quantum Dynamics" offers them an accessible introduction. Although the calculation of large systems still presents a challenge - despite the considerable power of modern computers - new strategies have been developed to extend the studies to systems of increasing size. Such strategies are presented after a brief overview of the historical background. Strong emphasis is put on an educational presentation of the fundamental concepts, so that the reader can inform himself about the most important concepts, like eigenstates, wave packets, quantum mechanical resonances, entanglement, etc. The chosen examples highlight that high-level experiments and theory need to work closely together. This book thus is a must-read both for researchers working experimentally or theoretically in the concerned fields, and generally for anyone interested in the exciting world of molecular quantum dynamics.



149,79 €

139,99 € (zzgl. MwSt.)

Lieferfrist: bis zu 10 Tage

Artikelnummer: 9783662512265

Medium: Buch

ISBN: 978-3-662-51226-5

Verlag: Springer

Erscheinungstermin: 23.08.2016

Sprache(n): Englisch

Auflage: Softcover Nachdruck of the original 1. Auflage 2014

Serie: Physical Chemistry in Action

Produktform: Kartoniert

Gewicht: 4336 g

Seiten: 273

Format (B x H): 155 x 235 mm

