

Molecular Quantum Dynamics



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(Dr. Davonte Schmidt MD)

MOLECULAR QUANTUM DYNAMICS



Springer Sep 2016, 2016. Taschenbuch. Book Condition: Neu. 235x155x15 mm. This item is printed on demand - Print on Demand Neuware - 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,...



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