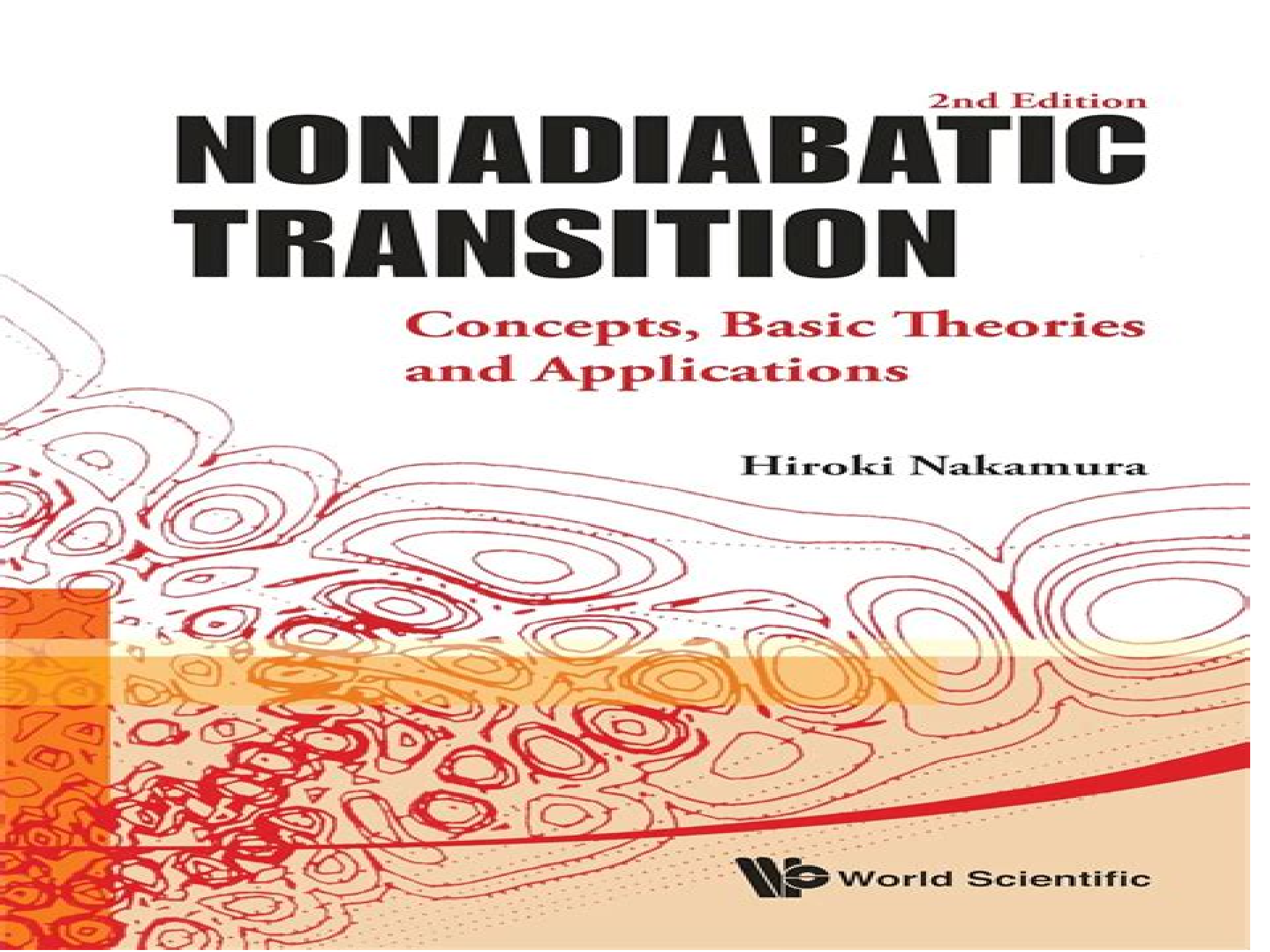




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Concepts, Basic Theories
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Nonadiabatic Transition: Concepts, Basic Theories And Applications (2nd Edition) Hiroki Nakamura, 2012-01-13

Nonadiabatic transition is a highly multidisciplinary concept and phenomenon constituting a fundamental mechanism of state and phase changes in various dynamical processes of physics chemistry and biology such as molecular dynamics energy relaxation chemical reaction and electron and proton transfer Control of molecular processes by laser fields is also an example of time dependent nonadiabatic transition In this new edition the original chapters are updated to facilitate enhanced understanding of the concept and applications Three new chapters comprehension of nonadiabatic chemical dynamics control of chemical dynamics and manifestation of molecular functions are also added

Introduction To Nonadiabatic Dynamics Hiroki Nakamura, 2019-09-26 Nonadiabatic transition is a highly multi disciplinary concept and phenomenon constituting a fundamental mechanism of state and phase changes in various dynamical processes of physics chemistry and biology This book is intended to be readable to a broad audience so that they can deepen their understanding of the basic concepts of both time independent and time dependent nonadiabatic transitions Quantum mechanically intriguing phenomena such as complete reflection and nonadiabatic tunneling are emphasized The Zhu Nakamura theory that can deal with non negligible classically forbidden transitions is explained Furthermore by controlling nonadiabatic transitions induced by an external field such as laser designing chemical reaction dynamics as we desire is shown to be theoretically possible

Laser Control Of Chemical Dynamics: With Emphasis On Nonadiabatic Transition Hiroki Nakamura, 2024-09-10 Laser control of chemical dynamics is one of the active research fields in molecular science brought about by significant advances in laser technology and further development of quantum control theory This monograph features the author's outstanding contributions to the field The first four chapters provide an excellent review of the fundamental subjects that are crucial to understanding laser molecule interactions with the highlight being his Zhu Nakamura theory of nonadiabatic transition This is an important basic theory for describing processes relevant to laser control and has been used by scientists around the world because of its simplicity and accuracy The remaining chapters propose theoretical possibilities of controlling various chemical dynamic processes based on theories discussed earlier in the book

The DV-X α Molecular-Orbital Calculation Method Tomohiko Ishii, Hisanobu Wakita, Kazuyoshi Ogasawara, Yang-Soo Kim, 2014-11-06 This multi author contributed volume contains chapters featuring the development of the DV X method and its application to a variety of problems in Materials Science and Spectroscopy written by leaders of the respective fields The volume contains a Foreword written by the Chairs of Japanese and Korea DV X alpha Societies This book is aimed at

individuals working in Quantum Chemistry The Non-Ergodic Nature of Internal Conversion Thomas Scheby Kuhlman, 2013-05-23 This thesis investigates the transitions from one electronically excited state to another Such processes the fastest of events in chemistry can be studied with femtosecond resolution and Thomas S Kuhlman approaches the question both with experimental and theoretical methods His approach contributes to explain processes of high importance to all scientific fields concerned with the interaction between light and matter the deactivation of the electronically excited states after excitation Thomas S Kuhlman concludes in this thesis that the electronic transition proceeds before the entire set of available degrees of freedom are active It is as simple as that **Ab Initio Molecular Dynamics** Dominik Marx, Jürg Hutter, 2009-04-30 Ab initio molecular dynamics revolutionized the field of realistic computer simulation of complex molecular systems and processes including chemical reactions by unifying molecular dynamics and electronic structure theory This book provides the first coherent presentation of this rapidly growing field covering a vast range of methods and their applications from basic theory to advanced methods This fascinating text for graduate students and researchers contains systematic derivations of various ab initio molecular dynamics techniques to enable readers to understand and assess the merits and drawbacks of commonly used methods It also discusses the special features of the widely used Car Parrinello approach correcting various misconceptions currently found in research literature The book contains pseudo code and program layout for typical plane wave electronic structure codes allowing newcomers to the field to understand commonly used program packages and enabling developers to improve and add new features in their code **Quantum Mechanical Tunneling in Chemical Physics** Hiroki Nakamura, Gennady Mil'nikov, 2016-04-19 Quantum mechanical tunneling plays important roles in a wide range of natural sciences from nuclear and solid state physics to proton transfer and chemical reactions in chemistry and biology Responding to the need for further understanding of multidimensional tunneling the authors have recently developed practical methods that can be applied to **Advances in Atomic, Molecular, and Optical Physics** , 2014-08-21 Advances in Atomic Molecular and Optical Physics publishes reviews of recent developments in a field that is in a state of rapid growth as new experimental and theoretical techniques are used on many old and new problems Topics covered include related applied areas such as atmospheric science astrophysics surface physics and laser physics Articles are written by distinguished experts and contain relevant review material and detailed descriptions of important recent developments International experts Comprehensive articles New developments **Computer Simulations in Condensed Matter: From Materials to Chemical Biology. Volume 2** Mauro Ferrario, Giovanni Ciccotti, Kurt Binder, 2007-04-16 This extensive and comprehensive collection of lectures by world leading experts in the field introduces and reviews all relevant computer simulation methods and their applications in condensed matter systems Volume 2 offers surveys on numerical experiments carried out for a great number of systems ranging from materials sciences to chemical biology including supercooled liquids spin glasses colloids polymers liquid crystals biological membranes and

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