Chemical Dynamics In Condensed Phases Relaxation Transfer And Reactions In Condensed Molecular Systems Oxford Graduate Texts

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Textbook on modern theoretical chemistry suitable for advanced undergraduate or graduate students.

The school held at Villa Marigola, Lerici, Italy, in July 1997 was very much an educational experiment aimed not just at teaching a new generation of students the latest developments in computer simulation methods and theory, but also at bringing together researchers from the condensed matter computer simulation community, the biophysical chemistry community and the quantum dynamics community to confront the shared problem: the development of methods to treat the dynamics of quantum condensed phase systems. This volume collects the lectures delivered there. Due to the focus of the school, the contributions divide along natural lines into two broad groups: (1) the most sophisticated forms of the art of computer simulation, including biased phase space sampling schemes, methods which address the multiplicity of time scales in condensed phase problems, and static equilibrium methods for treating quantum systems; (2) the contributions on quantum dynamics, including methods for mixing quantum and classical dynamics in condensed phase simulations and methods capable of treating all degrees of freedom quantum-mechanically. Contents:Barrier Crossing: Classical Theory of Rare but Important Events (D Chandler)Monte Carlo Simulations (D Frenkel)Molecular Dynamics Methods for the Enhanced Sampling of Phase Space (B J Berne)Constrained and Nonequilibrium Molecular Dynamics (G Ciccotti & M Ferrario)From Erying to Kramers: Computation of Diffusive Barrier Crossing Rates (M J Ruiz-Montero)Monte Carlo Methods for Sampling of Rare Event States (W Janke)Proton Transfer in Ice (D Marx)Nudged Elastic Band Method for Finding Minimum Energy Paths of Transitions (H Jónsson et al.)RAW Quantum Transition State Theory (G Mills et al.)Dynamics of Peptide Folding (R Elber et al.)Theoretical Studies of Activated Processes in Biological Ion Channels (B Roux & S Crouzy)The Semiclassical Initial Value Representation for Including Quantum Effects in Molecular Dynamics Simulations (W H Miller)Tunneling in the Condensed Phase: Barrier Crossing and Dynamical Control (N Makri)Feynman Path Centroid Methods for Condensed Phase Quantum Dynamics (G A Voth)Quantum Molecular Dynamics Using Wigner Representation (V S Filinov et al.)Nonadiabatic Molecular Dynamics Methods for Diffusion (D Laria et al.)and other papers Readership: Computational and statistical physicists. Keywords:Quantum;Molecular Dynamics;DynamicsReviews: “… this volume is a useful introduction to currently popular, and widely-used techniques in chemical and statistical physics. The authors are well-respected researchers in the field and the level is appropriate to graduate students and researchers.” Journal of Statistical Physics

Advanced graduate-level text looks at symmetry, rotations, and angular momentum addition; occupation number representations; and scattering theory. Uses concepts to develop basic theories of chemical reaction rates. Problems and answers.

Continuing the tradition of the Advances in Chemical Physics series, Volume 101: Chemical Reactions and Their Control on the Femtosecond Time Scale details the extraordinary findings reported at the XXth Solvay Conference on Chemistry, held at the Universite Libre de Bruxelles, Belgium, from November 28 to December 2, 1995. This new volume discusses the remarkable opportunities afforded by the femtosecond laser, focusing on the host of phenomena this laser has made it possible to observe. Examining molecules on the intrinsic time scale of their vibrations as well as their dissociative motions and electronic excitations represents only part of a broadened scientific window made possible by the femtosecond laser. The assembled studies, with follow-up discussions, reflect the many specialties and perspectives of the Conference's 65 participants as well as their optimism concerning the breadth of scientific discovery now open to them. The studies shed light on the laser's enhanced technical reach in the area of coherent control of chemical reactions as well as of more general quantum systems. The theoretical fundamentals of femto-chemistry, the unique behavior of the femtosecond laser, and a view toward future technological applications were also discussed: * Femtochemistry: chemical reaction dynamics and their control * Coherent control with femtosecond laser pulses * Femtosecond chemical dynamics in condensed phases * Control of quantum many-body dynamics * Experimental observation of laser control * Solvent dynamics and RRKM theory of clusters * High-resolution spectroscopy and intramolecular dynamics * Molecular Rydberg states and ZEKE spectroscopy * Transition-state spectroscopy and photodissociation * Quantum and semiclassical theories of chemical reaction rates. A fascinating and informative status report on the cutting-edge chemical research made possible by the femtosecond laser, Chemical Reactions and Their Control on the Femtosecond Time Scale is an indispensable volume for professionals and students alike. The femtosecond laser and chemistry's extraordinary new frontier of molecular motions observed on the scale of a quadrillionth of a second. Research chemists have only tapped the surface of the spectacular reach and precision of the femtosecond laser, a technology that has allowed them to observe the dynamics of molecules on the intrinsic time scale of their vibrations, dissociative motions, and electronic excitations. Volume 101 in the Advances in Chemical Physics series, Chemical Reactions and Their Control on the Femtosecond Time Scale details their extraordinary findings, presented at the XXth Solvay Conference on Chemistry, in Brussels. The studies reflect the work, in part, of the Conference's 65 participants, including many prominent contributors. Together they shed light on the laser's enhanced technical range in the area of coherent control of chemical reactions as well as of more general quantum systems. The theoretical fundamentals of femtochemistry, the unique behavior of the femtosecond laser, and a view toward future technological applications were also discussed. An exceptionally up-to-date examination of the chemical analyses made possible by the femtosecond laser, Chemical Reactions and Their Control on the Femtosecond Time Scale is an important reference for professionals and students interested in enhancing their research capabilities with this remarkable tool. From 1993 to 1996, she worked with Dr. P. Gaspard at the Universite Libre de Bruxelles, Belgium, on the application of new semiclassical techniques to elementary chemical reaction processes.

This 3rd edition has been expanded and updated to account for recent developments, while new illustrative examples as well as an enlarged reference list have also been added. It naturally retains the successful concept of its predecessors in presenting a unified perspective on molecular charge and energy transfer processes, thus bridging the regimes of coherent and dissipative dynamics, and establishing a connection between classic rate theories and modern treatments of ultrafast phenomena. Among the new topics are: - Time-dependent density functional theory - Heterogeneous electron transfer, e.g. between molecules and metal or semiconductor surfaces - Current flows through a single molecule. While serving as an introduction for graduate students and researchers, this is equally must-have reading for theoreticians and experimentalists, as well as an aid to interpreting experimental

data and accessing the original literature.

This volume presents an up-to-date overview of developments in the field of ultrafast reaction dynamics in condensed phases. Thirteen contributions, written by leading experts, report on a variety of chemical phenomena studied by many different experimental and theoretical techniques. Topics discussed include ultrafast spectroscopic techniques; aspects of electron transfer reactions ranging from solvent effects; intermolecular and intramolecular systems, to dynamics at semiconductor surfaces; the dynamics of chemical systems using Raman spectroscopy; pericyclic photochemical rearrangements and photodissociation reactions; solvent--solute interaction dynamics; and chemical dynamics in clusters. Theoretical treatments of impulsive femtosecond pump-probe spectroscopy, solvation dynamics and electron transfer are presented. The field of ultrafast chemistry is growing rapidly. The works described in this volume provide an overview of many of the exciting areas currently under study. For researchers interested in up-to-date theoretical and experimental developments in ultrafast spectroscopy in chemical systems.

Molecular simulation is a powerful tool in materials science, physics, chemistry and biomolecular fields. This updated edition provides a pragmatic introduction to a wide range of techniques for the simulation of molecular systems at the atomic level. The first part concentrates on methods for calculating the potential energy of a molecular system, with new chapters on quantum chemical, molecular mechanical and hybrid potential techniques. The second part describes methods examining conformational, dynamical and thermodynamical properties of systems, covering techniques including geometry-optimization, normal-mode analysis, molecular dynamics, and Monte Carlo simulation. Using Python, the second edition includes numerous examples and program modules for each simulation technique, allowing the reader to perform the calculations and appreciate the inherent difficulties involved in each. This is a valuable resource for researchers and graduate students wanting to know how to use atomic-scale molecular simulations. Supplementary material, including the program library and technical information, available through www.cambridge.org/9780521852524.

This volume describes many of the key practical theoretical techniques that have been developed to treat chemical dynamics problems in many-atom systems. It contains thorough treatments of fundamental theory and prescriptions for performing computations. The selection of methods, ranging from gas phase bimolecular reactions to complex processes in condensed phases, reflects the breadth of the field.The book is an excellent reference for proven and accepted methods as well as for theoretical approaches that are still being developed. It is appropriate for graduate students and other ?novices? who wish to begin working in chemical dynamics as well as active researchers who wish to acquire a wider knowledge of the field.

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.

Hydrogen bonds represent type of molecular interaction that determines the structure and function of a large variety of molecular systems. The elementary dynamics of hydrogen bonds and related proton transfer reactions, both occurring in the ultra fast time domain between 10-14 and 10-11s, form a research topic of high current interest. In this book addressing scientists and graduate students in physics, chemistry and biology, the ultra fast dynamics of hydrogen bonds and proton transfer in the condensed phase are reviewed by leading scientists, documenting the state of the art in this exciting field from the viewpoint of theory and experiment. The nonequilibrium behavior of hydrogen-bonded liquids and intramolecular hydrogen bonds as well as photo induced hydrogen and proton transfer are covered in 7 chapters, making reference to the most recent literature.

The main goal of this program is the development and application of computational methods for studying chemical reaction dynamics and molecular spectroscopy in the gas phase. We are interested in developing rigorous quantum dynamics algorithms for small polyatomic systems and in implementing approximate approaches for complex ones. Particular focus is on the dynamics and kinetics of chemical reactions and on the rovibrational spectra of species involved in combustion processes. This research also explores the potential energy surfaces of these systems of interest using state-of-the-art quantum chemistry methods, and extends them to understand some important properties of materials in condensed phases and interstellar medium as well as in combustion environments.

Significant accomplishments were made under the program of dynamical spectroscopy, aimed at elucidating details of chemical dynamics in condensed media. In fact, there now is a well-defined field of multi-dimensional spectroscopy, entirely aimed at the essence of what we had proposed. In the same natural vain of evolution, we developed the rather powerful technique of Time and Frequency Resolved Coherent Anti Stokes Raman Scattering (TFRCARS), as a tool that goes beyond the interrogation of interactions and molecular dynamics in condensed media. This four-wave mixing scheme, with transform limited detection of evolving coherences, can be regarded as a complete experiment in the creation, manipulation, and interrogation of quantum coherences. As such, it foreshadows useful quantum control, be it for chemical or computational purposes. A significant part of our present effort is aimed at devising and implementing control with shaped pulses to demonstrate computational algorithms in the laboratory. The original inspiration for developing TFRCARS was our aim to manipulate molecular wavepackets in regions where direct pumping could not be achieved, due to the inaccessible Franck-Condon factors. The target of those studies was the detailed dissection of non-adiabatic dynamics in the condensed phase prototype of solvated molecular iodine. While significant progress has been made toward this end, both direct experimentation and theoretical understanding of this process remain somewhat illusive. Highlights of advances made in theory and experiment are given based on some 20 published works that have appeared during this funding period, as a result of partial or total support by the grant.

The theoretical methods of quantum chemistry have matured to the point that accurate predictions can be made and experiments can be understood for a wide range of important gas-phase phenomena. A large part of this success can be attributed to the maturation of hierarchies of approximation, which allow one to approach very high accuracy, provided that sufficient computational resources are available. Until recently, these hierarchies have not been available in condensed-phase chemistry, but recent advances in the field have now led to a group of methods that are capable of reaching this goal. Accurate Condensed-Phase Quantum Chemistry addresses these new methods and the problems to which they can be applied. The book begins with an overview of periodic treatments of electron correlation, with an emphasis on the algorithmic features responsible for their computational efficiency. The first section of the book: Describes the Laplace-transform approach to periodic second-order perturbation theory (MP2) Examines local and density fitted schemes for MP2 in crystalline systems Presents test calculations for a variety of systems with small and medium-sized unit cells The next section focuses on methods based on treatment of the periodic solid in terms of fragments. This part of the book: Explores the incremental many-body scheme for electron correlation in solids, and describes progress towards metals and molecules on surfaces Describes the hierarchical method as an alternative fragment-based approach to electron correlation in crystalline solids, using conventional molecular electronic structure methods Examines electrostatically embedded many-body expansion for large systems, with an emphasis on molecular clusters and molecular liquids Explores

delocalized and localized orbital approaches to the electronic structures of periodic and non-periodic solids Lastly, the book describes a practical method by which conventional molecular electronic structure theory can be applied to molecular liquids and solids. Along with the methodology, it presents results on small to medium water clusters as well as on liquid water.

This study guide aims at explaining theoretical concepts encountered by practitioners applying theory to molecular science. This is a collection of short chapters, a manual, attempting to walk the reader through two types of topics: (i) those that are usually covered by standard texts but are difficult to grasp and (ii) topics not usually covered, but are essential for successful theoretical research. The main focus is on the latter. The philosophy of this book is not to cover a complete theory, but instead to provide a set of simple study cases helping to illustrate main concepts. The focus is on simplicity. Each section is made deliberately short, to enable the reader to easily grasp the contents. Sections are collated in themed chapters, and the advantage is that each section can be studied separately, as an introduction to more in-depth studies. Topics covered are related to elasticity, electrostatics, molecular dynamics and molecular spectroscopy, which form the foundation for many presently active research areas such as molecular biophysics and soft matter physics. The notes provide a uniform approach to all these areas, helping the reader to grasp the basic concepts from a common set of theoretical tools.

Thanks to the progress made in instruments and techniques, the methods in physical chemistry have developed rapidly over the past few decades, making them increasingly valuable for scientists of many disciplines. These two must-have volumes meet the needs of the scientific community for a thorough overview of all the important methods currently used. As such, this work bridges the gap between standard textbooks and review articles, covering a large number of methods, as well as the motivation behind their use. A uniform approach is adopted throughout both volumes, while the critical comparison of the advantages and disadvantages of each method makes this a valuable reference for physical chemists and other scientists working with these techniques.

Electron Transfer in Chemistry and Biology An Introduction to the Theory Alexander M. Kuznetsov Russian Academy of Sciences, Moscow, Russia Jens Ulstrup Technical University of Denmark, Lyngby, Denmark Electron transfer is perhaps the single most important physical event in chemical, electrochemical, photochemical, biochemical, and biophysical processes. The focus and ubiquity of electron transfer is intriguing and exciting but a coherent and comprehensive approach to this topic is at the same time a challenge. Electron Transfer in Chemistry and Biology provides a thorough and didactic approach to the theoretical basis of electron transfer phenomena. Not only does it offer a full introduction to this area and a discussion of its historical development, it also gives detailed explanations of difficult issues, for example, long-range electron transfers, stochastic and dynamic processes, and biological features. A wide variety of readers will find this volume of great interest, ranging from final year undergraduate students, postgraduate students and university lecturers, to research staff in numerous fields including medical companies, electronics industry, catalysis research and development, chemical industry and some hospitals.

Complex systems that bridge the traditional disciplines of physics, chemistry, biology, and materials science can be studied at an unprecedented level of detail using increasingly sophisticated theoretical methodology and high-speed computers. The aim of this book is to prepare burgeoning users and developers to become active participants in this exciting and rapidly advancing research area by uniting for the first time, in one monograph, the basic concepts of equilibrium and time-dependent statistical mechanics with the modern techniques used to solve the complex problems that arise in real-world applications. The book contains a detailed review of classical and quantum mechanics, in-depth discussions of the most commonly used ensembles simultaneously with modern computational techniques such as molecular dynamics and Monte Carlo, and important topics including free-energy calculations, linear-response theory, harmonic baths and the generalized Langevin equation, critical phenomena, and advanced conformational sampling methods. Burgeoning users and developers are thus provided firm grounding to become active participants in this exciting and rapidly advancing research area, while experienced practitioners will find the book to be a useful reference tool for the field.

Brings Readers from the Threshold to the Frontier of Modern Research Many-Body Methods for Atoms and Molecules addresses two major classes of theories of electron correlation: the many-body perturbation theory and coupled cluster methods. It discusses the issues related to the formal development and consequent numerical implementation of the methods from the standpoint of a practicing theoretician. The book will enable readers to understand the future development of state-of-the-art multi-reference coupled cluster methods as well as their perturbative counterparts. The book begins with an introduction to the issues relevant to the development of correlated methods in general. It next gives a formally rigorous treatment of aspects that pave the foundation toward the theoretical development of methods capable of tackling problems of electronic correlation. The authors go on to cover perturbation theory first in a fundamental way and then in the multi-reference context. They also describe the idea of state-specific theories, Fock space-based multi-reference coupled cluster methods, and basic issues of the single-reference coupled cluster method. The book concludes with state-of-the-art methods of modern electronic structure.

This book is meant to provide a window on the rapidly growing body of theoretical studies of condensed phase chemistry. A brief perusal of physical chemistry journals in the early to mid 1980’s will find a large number of theor- ical papers devoted to 3-body gas phase chemical reaction dynamics. The recent history of theoretical chemistry has seen an explosion of progress in the devel- ment of methods to study similar properties of systems with Avogadro’s number of particles. While the physical properties of condensed phase systems have long been principle targets of statistical mechanics, microscopic dynamic theories that start from detailed interaction potentials and build to first principles predictions of properties are now maturing at an extraordinary rate. The techniques in use range from classical studies of new Generalized Langevin Equations, semicl- sical studies for non-adiabatic chemical reactions in condensed phase,

mixed quantum classical studies of biological systems, to fully quantum studies of m- els of condensed phase environments. These techniques have become sufficiently sophisticated, that theoretical prediction of behavior in actual condensed phase environments is now possible. and in some cases, theory is driving development in experiment. The authors and chapters in this book have been chosen to represent a wide variety in the current approaches to the theoretical chemistry of condensed phase systems. I have attempted a number of groupings of the chapters, but the - versity of the work always seems to frustrate entirely consistent grouping.

Graduate level textbook presenting some of the most fundamental processes that underlie physical, chemical and biological phenomena in complex condensed phase systems. Includes in-depth descriptions of relevant methodologies, and provides ample introductory material for readers of different backgrounds.

A guide to the theoretical and computational toolkits for the modern study of molecular kinetics in condensed phases Molecular Kinetics in Condensed Phases: Theory, Simulation and Analysis puts the focus on the theory, algorithms, simulations methods and analysis of molecular kinetics in condensed phases. The authors – noted experts on the topic – offer a detailed and thorough description of modern theories and simulation methods to model molecular events. They highlight the rigorous stochastic modelling of molecular processes and the use of mathematical models to reproduce experimental observations, such as rate coefficients, mean first passage times and transition path times. The book's exploration of simulations examines atomically detailed modelling of molecules in action and the connections of these simulations to theory and experiment. The authors also explore the applications that range from simple intuitive examples of one- and two-dimensional systems to complex solvated macromolecules. This important book: Offers an introduction to the topic that combines theory, simulation and analysis Presents a guide written by authors that are well-known and highly regarded leaders in their fields Contains detailed examples and explanation of how to conduct computer simulations of kinetics. A detailed study of a two-dimensional system and of a solvated peptide are discussed. Discusses modern developments in the field and explains their connection to the more traditional concepts in chemical dynamics Written for students and academic researchers in the fields of chemical kinetics, chemistry, computational statistical mechanics, biophysics and computational biology, Molecular Kinetics in Condensed Phases is the authoritative guide to the theoretical and computational toolkits for the study of molecular kinetics in condensed phases.

The Advances in Chemical Physics series provides the chemical physics and physical chemistry fields with a forum for critical, authoritative evaluations of advances in every area of the discipline. Filled with cutting-edge research reported in a cohesive manner not found elsewhere in the literature, each volume of the Advances in Chemical Physics series serves as the perfect supplement to any advanced graduate class devoted to the study of chemical physics.

This series of volumes aims to publish authoritative review articles on a wide range of exciting and contemporary topics in gas and condensed phase kinetics. Research in Chemical Kinetics complements the acclaimed series Comprehensive Chemical Kinetics, and is edited by the same team of professionals. The reviews contained in this volume are concise, topical accounts of specific research written by acknowledged experts. The authors summarize their latest work and place it in a general context. Particular strengths of the volume are the quality of the contributions and their topicality, and the rapid publication realized.

Physical Chemistry: An Advanced Treatise: Reactions in Condensed Phases, Volume VII, deals with reactions in condensed phases. The purpose of this treatise is to present a comprehensive treatment of physical chemistry for advanced students and investigators in a reasonably small number of volumes. An attempt has been made to include all important topics in physical chemistry together with borderline subjects which are of particular interest and importance. The book begins by discussing the basic principles of reaction rates in solution. This is followed by separate chapters on estimating the rate parameters of elementary reactions; the use of correlation diagrams to interpret organic reactions; perturbation of reaction rates by substituents; and inorganic reactions. Subsequent chapters cover the important field of free radicals, including chain reactions and solvent effects; heterogeneous catalysis; various types of surface reactions; surface annealing; electron reactions; nucleation; and radiation chemistry. The book presents a broad picture of current developments in reaction rates in condensed phases in a form accessible to all students of chemical kinetics. This treatment, by experts in widely different areas, will hopefully meet many student needs and provide a useful overview for all.

The Twenty Sixth Jerusalem Symposium reflected the high standards of these distinguished scientific meetings, which convene once a year at the Israel Academy of Sciences and Humanities in Jerusalem to discuss a specific topic in the broad area of quantum chemistry and biochemistry. The topic at this year's Jerusalem Symposium was reaction dynamics in clusters and condensed phases, which constitutes a truly interdisciplinary subject of central interest in the areas of chemical dynamics, kinetics, photochemistry and condensed matter chemical physics. The main theme of the Symposium was built around the exploration of the interrelationship between the dynamics in large finite clusters and in infinite bulk systems. The main issues addressed microscopic and macroscopic sol vation phenomena, cluster and bulk spectroscopy, photodissociation and vibrational predissociation, cage effects, interphase dynamics, reaction dynamics and energy transfer in clusters, dense fluids, liquids, solids and biophysical systems. The interdisciplinary nature of this research area was deliberated by intensive and extensive interactions between modern theory and advanced experimental methods. This volume provides a record of the invited lectures at the Symposium.

Macromolecular materials possess some remarkable features arising from the fact that their molecules are made up of more or less flexible chains which can have various conformations. The study of molecular conformations and dynamics of macromolecules is important in polymer science and technology from both basic and practical viewpoints. In practice, these studies have concentrated on dilute solutions but more recently there has been a clear trend towards studying molecular properties in condensed systems in order to understand the entire macromolecular system based on a unified concept. Based on lectures presented by an internationally recognized group of polymer scientists at a meeting held in Japan in October 1987 (plus two additional contributions), this volume summarises present knowledge of molecular conformations and dynamics of macromolecules from dilute solutions to various condensed systems. The book is not a random collection of papers of the usual conference proceedings type. Authors prepared their contributions in line with an overall plan for the work, were able to discuss the content with colleagues at the meeting, and finalised their text after the conference. It is thus a comprehensive, integrated overview of the field. Current developments in both theory and experiment are discussed in a well-balanced way. The behaviour of macromolecules at phase transition and interface is discussed in relation to their behaviour in bulk systems. The book offers a particularly up-to-date and authoritative picture of the current state of the art, and will be of interest to all research and professional workers concerned with polymer science in universities, industry, and government institutions.

The book is divided in two parts, to supply first the basic elements of the language, with short but complete explanations of terms, methods and theories; and then to describe the present status of studies on the processes by which organic molecules aggregate to form observable bodies and to determine their physical and chemical properties.

This book highlights the latest experimental and theoretical developments in the field of femtochemistry, with papers describing the physics and chemistry of ultrafast processes in small molecules, complex molecular systems, clusters, biological systems, solids, matrices, liquids and at surfaces and interfaces. The recent developments in frequency-

domain studies of femtodynamics are also presented. In addition, the latest achievements in femtosecond control of chemical reactions are presented, together with the newest techniques in real-time probing of reactions such as ultrafast x-ray or electron diffraction. The papers are rich in references giving a clearcut state-of-the-art of the topics being discussed. The book should be a valuable tool to all persons in the field and to young scientists. Contributors include: A H Zewail, J Jortner, V S Letokhov, J Manz, R S Berry, C Wittig, K B Eisenthal, A W Castleman Jr., J T Hynes, W H Gadzuk, R Kosloff, S Mukamel, K R Wilson; G Fleming, D Wiersma, K Yoshihara, V Sundström, A Apkarian, N Scherer, A Myers, R Schinke, J R Huber, R B Gerber, G Gerber and P M Champion. Contents:Keynote and Overview PapersElementary ReactionsComplex Molecular SystemsClustersFemtodynamics from SpectroscopyControl; Biological SystemsSurfaces and InterfacesLiquidsSolids and MatricesTechniques and Methods Readership: Chemists, physicists, biophysicists and materials scientists. keywords:

This book deals with a central topic at the interface of chemistry and physics - the understanding of how the transformation of matter takes place at the atomic level. Building on the laws of physics, the book focuses on the theoretical framework for predicting the outcome of chemical reactions. The style is highly systematic with attention to basic concepts and clarity of presentation. Molecular reaction dynamics is about the detailed atomic-level description of chemical reactions. Based on quantum mechanics and statistical mechanics or, as an approximation, classical mechanics, the dynamics of uni- and bi-molecular elementary reactions are described. The book features a detailed presentation of transition-state theory which plays an important role in practice, and a comprehensive discussion of basic theories of reaction dynamics in condensed phases. Examples and end-of-chapter problems are included in order to illustrate the theory and its connection to chemical problems.

Chemistry at Extreme Conditions covers those chemical processes that occur in the pressure regime of 0.5–200 GPa and temperature range of 500–5000 K and includes such varied phenomena as comet collisions, synthesis of super-hard materials, detonation and combustion of energetic materials, and organic conversions in the interior of planets. The book provides an insight into this active and exciting field of research. Written by top researchers in the field, the book covers state of the art experimental advances in high-pressure technology, from shock physics to laser-heating techniques to study the nature of the chemical bond in transient processes. The chapters have been conventionally organised into four broad themes of applications: biological and bioinorganic systems; Experimental works on the transformations in small molecular systems; Theoretical methods and computational modeling of shock-compressed materials; and experimental and computational approaches in energetic materials research. * Extremely practical book containing up-to-date research in high-pressure science * Includes chapters on recent advances in computer modelling * Review articles can be used as reference guide

Exploring recent developments in the field, Coarse-Graining of Condensed Phase and Biomolecular Systems examines systematic ways of constructing coarse-grained representations for complex systems. It explains how this approach can be used in the simulation and modeling of condensed phase and biomolecular systems. Each chapter focuses on specific examples of evolving coarse-graining methodologies and presents results for a variety of complex systems. The contributors carefully detail their own coarse-graining approach, exploring its motivation, strengths, weaknesses, and important application examples. They discuss two of the most successful coarse-graining schemes for soft matter: inverse and multiscale coarse-graining. The book also describes current coarse-grained model development for peptides and proteins at the amino acid level and larger length scales. Assembling the work of some of the most influential, world-renowned researchers in the field, this book provides a unified, in-depth overview of all the coarse-grained schemes developed for condensed phase and biomolecular systems. It shows the promise of coarse-graining as a revolutionary advancement in the scientific community.

This book highlights the need for studying multi-state models analytically for understanding the physics of molecular processes. An intuitive picture about recently solved models of statistical and quantum mechanics is drawn along with presenting the methods developed to solve them. The models are relevant in the context of molecular processes taking place in gaseous phases and condensed phases, emphasized in the introduction. Chapter 1 derives the arisal of multi-state models for molecular processes from the full Hamiltonian description. The model equations are introduced and the literature review presented in short. In Chapter 2, the time-domain methods to solve Smoluchowski-based reaction-diffusion systems with single-state and two-state descriptions are discussed. Their corresponding analytical results derive new equilibrium concepts in reversible reactions and studies the effect of system and molecular parameters in condensed-phase chemical dynamics. In Chapter 3, time-domain methods to solve quantum scattering problems are developed. Along side introducing a brand new solvable model in quantum scattering, it discusses transient features of quantum two-state models. In interest with electronic transitions, a new solvable two-state model with localized non-adiabatic coupling is also presented. The book concludes by proposing the future scope of the model, thereby inviting new research in this fundamentally important and rich applicable field.?