Molecular Vibration Dynamics In Molecule Surface Interactions

Femtosecond Dynamics of Molecules in the Condensed PhaseUltrafast Infrared Vibrational SpectroscopyQuantum Mechanics in ChemistryMolecular Quantum DynamicsMolecular Reaction DynamicsHandbook of SpectroscopySpectroscopic and Dynamic Studies of Highly Vibrationally Excited MoleculesPhysics BriefsDynamics of Molecules and Chemical ReactionsSpectroscopy of Biological Molecules: Modern TrendsClassical and Quantum Mechanical Studies of Molecular Vibrations for Triatomic MoleculesThe Molecular Dynamics of Liquid CrystalsSpectroscopy of Emerging MaterialsThe Future of Dynamic Structural ScienceControlled Synthesis of Nanoparticles in Microheterogeneous SystemsSpectroscopy and Dynamics of Single MoleculesNonlinearity and Chaos in Molecular VibrationsTheory of Chemical Reaction DynamicsState Selected and State to State Ion Molecule Reaction Dynamics, Part 2High Enthalpy Gas DynamicsAdvances in Molecular Vibrations and Collision DynamicsSpectra and Dynamics of Small MoleculesAdvances in Theoretically Interesting MoleculesNovel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and SimulationsBaltimore Lectures on Molecular Dynamics and the Wave Theory of LightDynamics of Molecule Surface InteractionDielectric Relaxation and Dynamics

of Polar MoleculesVibration-rotational Spectroscopy and Molecular DynamicsCoherent Vibrational DynamicsAirglow as an Indicator of Upper Atmospheric Structure and DynamicsThe Spectra and Dynamics of Diatomic MoleculesDynamics of Gas-Surface InteractionsThe Spectra and Dynamics of Diatomic MoleculesAttosecond and XUV PhysicsLow-Energy Electron Scattering from Molecules, Biomolecules and SurfacesThe Theory of Chemical Reaction DynamicsJet Spectroscopy and Molecular DynamicsProceedings of the International Conference of Computational Methods in Sciences and Engineering 2003 (ICCMSE 2003)Numerical Hamiltonian ProblemsCoherent Dynamics of Small Molecules in Rare Gas Crystals

Femtosecond Dynamics of Molecules in the Condensed Phase

Ultrafast Infrared Vibrational Spectroscopy

Advanced text explores mathematical problems that occur frequently in physics and other sciences. Topics include symplectic integration, symplectic order conditions, available symplectic methods, numerical experiments, properties of symplectic integrators. 1994 edition.

Quantum Mechanics in Chemistry

Includes bibliographical references.

Molecular Quantum Dynamics

And concluding with some examples of polyatomic molecule dynamics. P Students will discover that there is a fascinating world of cause-and-effect localized dynamics concealed beyond the reduction of spectra to archival molecular constants and the exact ab initio computation of molecular properties.-

Molecular Reaction Dynamics

These seven lectures are intended to serve as an introduction for beginning graduate students to the spectra of small molecules. The author succeeds in illustrating the concepts by using language and metaphors that capture and elegantly convey simple insights into dynamics that lie beyond archival molecular constants. The lectures can simultaneously be viewed as a collection of interlocking special topics that have fascinated the author and his students over the years. Though neither a textbook nor a scholarly monograph, the book provides an illuminating perspective that will benefit students and researchers alike.

Handbook of Spectroscopy

The book summarizes international progress over the last few decades in upper atmosphere airglow research. Measurement methods, theoretical concepts and empirical models of a wide spectrum of

upper atmospheric emissions and their variability are considered. The book contains a detailed bibliography of studies related to the upper atmosphere airglow. Readers will also benefit from a lot of useful information on emission characteristics and its formation processes found the book.

Spectroscopic and Dynamic Studies of Highly Vibrationally Excited Molecules

This is an introductory level textbook which explains the elements of high temperature and high-speed gas dynamics. written in a clear and easy to follow style, the author covers all the latest developments in the field including basic thermodynamic principles, compressible flow regimes and waves propagation in one volume covers theoretical modeling of High Enthalpy Flows, with particular focus on problems in internal and external gas-dynamic flows, of interest in the fields of rockets propulsion and hypersonic aerodynamics High enthalpy gas dynamics is a compulsory course for aerospace engineering students and this book is a result of over 25 years' teaching by the author accompanying website includes a Solutions Manual for exercises listed at the end of each chapter, plus lecture slides

Physics Briefs

This book gives a representative survey of the state of the art of research on gas-surface interactions. It provides an overview of the current understanding of gas surface dynamics and, in particular, of the

reactive and non-reactive processes of atoms and small molecules at surfaces. Leading scientists in the field, both from the theoretical and the experimental sides, write in this book about their most recent advances. Surface science grew as an interdisciplinary research area over the last decades, mostly because of new experimental technologies (ultra-high vacuum, for instance), as well as because of a novel paradigm, the 'surface science' approach. The book describes the second transformation which is now taking place pushed by the availability of powerful quantum-mechanical theoretical methods implemented numerically. In the book, experiment and theory progress hand in hand with an unprecedented degree of accuracy and control. The book presents how modern surface science targets the atomic-level understanding of physical and chemical processes at surfaces, with particular emphasis on dynamical aspects. This book is a reference in the field.

Dynamics of Molecules and Chemical Reactions

This work focuses on complementary crystallographic and spectroscopic areas of dynamic structural science, from papers presented at the 46th NATO sponsored course in Erice, Sicily 2013. These papers cover a range of material from background concepts to more advanced material and represent a fully inter-disciplinary collection of the latest ideas and results within the field. They will appeal to practising or novice crystallographers, both chemical and

biological, who wish to learn more about modern spectroscopic methods and convergent advances and hence vice versa for experimental and computational spectroscopists. The chapters refer to the latest techniques, software and results and each chapter is fully referenced. The volume provides an excellent starting point for new comers in the emerging, multi-disciplinary area of time resolved science.

Spectroscopy of Biological Molecules: Modern Trends

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.

Classical and Quantum Mechanical Studies of Molecular Vibrations for Triatomic Molecules

Chemical reactions at surfaces do not follow the same reaction dynamics as atoms in the gas phase. The changes from "ideal" interactions depend on the electronic structure and the spatial and geometric shape of the surface. The dynamics of chemical reactions at surfaces have all the complexity of gas-phase molecules reaction dynamics, plus those associated with the additional phenomena due to the presence of a solid surface.

The Molecular Dynamics of Liquid Crystals

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.

Spectroscopy of Emerging Materials

The Future of Dynamic Structural Science

Controlled Synthesis of Nanoparticles in Microheterogeneous Systems

In the past few decades, many significant insights have been gained into several areas of computational methods in sciences and engineering. New problems and methodologies have appeared in some areas of sciences and engineering. There is always a need in these fields for the advancement of information exchange. The aim of this book is to facilitate the sharing of ideas, problems and methodologies between computational scientists and engineers in several disciplines. Extended abstracts of papers on the recent advances regarding computational methods in sciences and engineering are provided. The book briefly describes new methods in numerical analysis, computational mathematics, computational and theoretical physics, computational and theoretical chemistry, computational biology, computational mechanics, computational engineering, computational medicine, high performance computing, etc.

Spectroscopy and Dynamics of Single Molecules

This second, thoroughly revised, updated and enlarged edition provides a straightforward introduction to spectroscopy, showing what it can do and how it does it, together with a clear, integrated and objective account of the wealth of information that may be derived from spectra. It also features new chapters on spectroscopy in nano-dimensions, nano-optics, and polymer analysis. Clearly structured into sixteen sections, it covers everything from spectroscopy in nanodimensions to medicinal applications, spanning a wide range of the electromagnetic spectrum and the physical processes involved, from nuclear phenomena to molecular rotation processes. In addition, data tables provide a comparison of different methods in a standardized form, allowing readers to save valuable time in the decision process by avoiding wrong turns, and also help in selecting the instrumentation and performing the experiments. These four volumes are a must-have companion for daily use in every lab.

Nonlinearity and Chaos in Molecular Vibrations

Covers both molecular and reaction dynamics. The work presents important theroetical and computational approaches to the study of energy transfer within and between molecules, discussing the application of these approaches to problems of experimental interest. It also describes time-dependent and time-independent methods, variational and perturbative techniques, iterative and direct approaches, and methods based upon the use

of physical grids of finite sets of basic function.

Theory of Chemical Reaction Dynamics

The 1997 European Conference on Spectroscopy of Biological Molecules (ECSBM) is the seventh in a biennial series of conferences devoted to the applications of molecular spectroscopy to biological molecules and related systems. The interest of these conferences rests mainly on the relationship between the structure and physiological activity of biological molecules and related systems of which these molecular species form part. This volume ofECSBM contains articles prepared by the invited lecturers and those making poster presentations at the seventh ECSBM. The reader will find mainly applications of vibrational spectroscopy to protein structure and dynamics, biomembranes, molecular recognition, nucleic acids and other biomolecules and biological systems containing specific chromophors. Biomedical applications of vibrational spectroscopy are expanding rapidly. On the other hand, a significant number of the papers describe applications of other methods, such as NMR, circular dichroism, optical absorption and fluorescence, X-ray absorption and diffraction and other theoretical methods. One aim has been to achieve a well balanced, critically comparative review of recent progress in the field of biomolecular structure, bonding and dynamics based on applications of the above spectroscopic methods. A great part of the contributions included in this volume are devoted to biomedical and biotechnological applications and provide a broadly

based account of recent applicationS in this field. The content of this book has been organized in sections corresponding mainly to the different types of biological molecules investigated. This book includes also another section related to theoretical methods where MO calculations of vibrational frequencies dominate clearly the topic.

State Selected and State to State Ion Molecule Reaction Dynamics, Part 2

The calculation of cross sections and rate constants for chemical reactions in the gas phase has long been a major problem in theoretical chemistry. The need for reliable and applicable theories in this field is evident when one considers the significant recent advances that have been made in developing experimental techniques, such as lasers and molecular beams, to probe the microscopic details of chemical reactions. For example, it is now becoming possible to measure cross sections for chemical reactions state selected in the vibrational rotational states of both reactants and products. Furthermore, in areas such as atmospheric, combustion and interstellar chemistry, there is an urgent need for reliable reaction rate constant data over a range of temperatures, and this information is often difficult to obtain in experiments. The classical trajectory method can be applied routinely to simple reactions, but this approach neglects important quantum mechanical effects such as tunnelling and resonances. For all these reasons, the quantum theory of reactive scattering is an area that has received considerable

attention recently. This book describes the proceedings of a NATO Advanced Research Workshop held at CECAM, Orsay, France in June, 1985. The Workshop concentrated on a critical examination and discussion of the recent developments in the theory of chemical reaction dynamics, with particular emphasis on quantum theories. Several papers focus on exact theories for reactions.

High Enthalpy Gas Dynamics

Nonlinearity and Chaos in Molecular Vibrations deals systematically with a Lie algebraic approach to the study of nonlinear properties of molecular highly excited vibrations. The fundamental concepts of nonlinear dynamics such as chaos, fractals, quasiperiodicity, resonance, and the Lyapunov exponent, and their roles in the study of molecular vibrations are presented. The 20 chapters cover the basic ideas, the concept of dynamical groups, the integrable two-mode SU(2) system, the unintegrable three-mode SU(3) system, the noncompact su(1,1) algebraic application, su(3) symmetry breaking and its application and the quantal effect of asymmetric molecular rotation. Emphasis is given to: resonance and chaos, the fractal structure of eigencoefficients, the C-H bend motion of acetylene, regular and chaotic motion of DCN, the existence of approximately conserved quantum numbers, one-electronic motion in multi-sites, the Lyapunov exponent, actions of periodic trajectories and quantization, the H function and its application in vibrational relaxation as well as the Dixon dip and its destruction and chaos in the

transitional states. This approach bridges the gap between molecular vibrational spectroscopy and nonlinear dynamics. The book presents a framework of information that readers can use to build their knowledge, and is therefore highly recommended for all those working in or studying molecular physics, molecular spectroscopy, chemical physics and theoretical physics. * Discusses nonlinearity and chaotic phenomena in molecular vibrations * Approaches the complicated highly excited molecular vibration * Provides clear information for students and researchers looking to expand knowledge in this field

Advances in Molecular Vibrations and Collision Dynamics

Spectra and Dynamics of Small Molecules

Because of their structural and dynamical properties, microheterogeneous systems have been employed as solvent and reaction media both to synthesize and stabilize nanoparticles. Following this route, inside their nanometer-sized heterogeneities the nanoparticles of many different substances have been incorporated. The book shows the distinct advantages of this synthetic strategy over that of many other methods. Moreover, it furnishes to the reader a collection of theoretical and experimental facts allowing him to reduce the number of trial and errors necessary to arrive at an optimal synthetic protocol.

Advances in Theoretically Interesting Molecules

Novel Approaches to the Structure and Dynamics of Liquids: Experiments, Theories and Simulations

The book reviews the results of vibration-rotational spectroscopy of molecules obtained recently by combining modern computational methods of quantum chemistry with the new techniques of high-resolution rotational and vibration-rotational spectroscopy. It shows for example that the tunneling vibration-rotational spectroscopy of the van der Waals complexes provides a new look at intermolecular forces while the high precision and sensitivity of the submillimeter-wave and Fourier transform microwave spectroscopy make it possible to study complex rotational spectra of molecules in excited vibrational states. New results of high level ab initio quantum chemical computations of vibrational and rotational energy levels and dipole moment functions of unusual molecules will be discussed together with the recent discovery of clustering of energy levels in asymmetric tops. Group theoretical analysis of floppy molecules, especially the tunneling effects in nonrigid molecules, will also be discussed.

Baltimore Lectures on Molecular Dynamics and the Wave Theory of Light

The advent of laser-based sources of ultrafast infrared pulses has extended the study of very fast molecular dynamics to the observation of processes manifested through their effects on the vibrations of molecules. In addition, non-linear infrared spectroscopic techniques make it possible to examine intra- and intermolecular interactions and how such interactions evolve on very fast time scales, but also in some instances on very slow time scales. Ultrafast Infrared Vibrational Spectroscopy is an advanced overview of the field of ultrafast infrared vibrational spectroscopy based on the scientific research of the leading figures in the field. The book discusses experimental and theoretical topics reflecting the latest accomplishments and understanding of ultrafast infrared vibrational spectroscopy. Each chapter provides background, details of methods, and explication of a topic of current research interest. Experimental and theoretical studies cover topics as diverse as the dynamics of water and the dynamics and structure of biological molecules. Methods covered include vibrational echo chemical exchange spectroscopy, IR-Raman spectroscopy, time resolved sum frequency generation, and 2D IR spectroscopy. Edited by a recognized leader in the field and with contributions from top researchers, including experimentalists and theoreticians, this book presents the latest research methods and results. It will serve as an excellent resource for those new to the field, experts in the field, and individuals who want to gain an understanding of particular methods and research topics.

Dynamics of Molecule Surface Interaction

Since the turn of the 21st century, the field of electron molecule collisions has undergone a renaissance. The importance of such collisions in applications from radiation chemistry to astrochemistry has flowered, and their role in industrial processes such as plasma technology and lighting are vital to the advancement of next generation devices. Furthermore, the development of the scanning tunneling microscope highlights the role of such collisions in the condensed phase, in surface processing, and in the development of nanotechnology. Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces highlights recent progress in the theory and experiment of electron-molecule collisions, providing a detailed review of the current state of knowledge of electron molecule scattering—theoretical and experimental—for the general physicist and chemist interested in solving practical problems. In few other branches of science is the collaboration between theorists and experimentalists so topical. Covering advancements in practical problems, such as those met in plasma physics, microelectronics, nanolithography, DNA research, atmospheric chemistry, and astrochemistry, this book describes the formal general scattering theory and description of the experimental setup at a level the interested non-expert can appreciate.

Dielectric Relaxation and Dynamics of

Polar Molecules

Remarkable developments in the spectroscopy field regarding ultrashort pulse generation have led to the possibility of producing light pulses ranging from 50 to5 fs and frequency tunable from the near infrared to the ultraviolet range. Such pulses enable us to follow the coupling of vibrational motion to the electronic transitions in molecules and solids in real time. Detailing these advanced developments, as well as the fundamental methods and tools of vibrational spectroscopy, Coherent Vibrational Dynamics providesresearchers and students with a uniquely comprehensive resource. With the contributions of pioneering scientists, this seminal volume – · Outlines the principles and tools used on time-domain vibrational spectroscopy and provides a general introduction to the subject of coherent phonons · Describes the modern methods for tunable ultrashort pulse generation from infrared to visible-UV · Reviews coherent vibrational dynamics in small molecules in liquids (hydrogen bonds), and in carbon based conjugated materials (polyenes, carotenoids, and semiconducting polymers) · Explores phonon dynamics in semiconductors (bulk and heterostructures) and in quasi-one-dimensional systems Supplemented with a great number of references, and covering fundamental as well advanced topics, this text provides a valuable reference for both graduate students and senior researchers investigating materials in physics, chemistry, and biology. It is also an excellent starting point for those who want to pursue research in the

field of ultrafast optics and spectroscopy.

Vibration-rotational Spectroscopy and Molecular Dynamics

This volume focuses on molecular clusters, bound by van der Waals interactions and hydrogen bonds. Twelve chapters review a wide range of recent theoretical and experimental advances in the areas of cluster vibrations, spectroscopy, and reaction dynamics. The authors are leading experts, who have made significant contributions to these topics. The first chapter describes exciting results and new insights in the solvent effects on the short-time photo fragmentation dynamics of small molecules, obtained by combining heteroclusters with femtosecond laser excitation. The second is on theoretical work on effects of single solvent (argon) atom on the photodissociation dynamics of the solute H2O molecule. The next two chapters cover experimental and theoretical aspects of the energetics and vibrations of small clusters. Chapter 5 describes diffusion quantum Monte Carlo calculations and non additive three-body potential terms in molecular clusters. The next six chapters deal with hydrogen-bonded clusters, reflecting the ubiquity and importance of hydrogen-bonded networks. The final chapter provides the microscopic theory of the dynamics and spectroscopy of doped helium cluster, highly quantum systems whose unusual properties have been studied extensively in the past couple of years.

Coherent Vibrational Dynamics

Recent years have seen an explosion in the volume of work carried out using supersonic jets of molecules following the discovery that the technique could provide information on structure and dynamics of a very high quality otherwise impossible to obtain. Written and edited by a first class team of authors, acknowledged world leaders in their subjects, this book describes applications in detail along with analysis of data recorded and background theory. Physical chemists and chemical physicists will find this unique book an essential concentrated source of information and reference.

Airglow as an Indicator of Upper Atmospheric Structure and Dynamics

Spectroscopy and Dynamics of Single Molecules: Methods and Applications reviews the most recent developments in spectroscopic methods and applications. Spectroscopic techniques are the chief experimental methods for testing theoretical models and research in this area plays an important role in stimulating new theoretical developments in physical chemistry. This book provides an authoritative insight into the latest advances in the field, highlighting new techniques, current applications, and potential future developments An ideal reference for chemists and physicists alike, Spectroscopy and Dynamics of Single Molecules: Methods and Applications is a useful guide for all those working in the research, design, or application of spectroscopic tools and techniques

across a wide range of fields. Includes the latest research on ultrafast vibrational and electronic dynamics, nonlinear spectroscopies, and single-molecule methods Makes the content accessible to researchers in chemistry, biophysics, and chemical physics through a rigorous multi-disciplinary approach Provides content edited by a world-renowned chemist with more than 30 years of experience in research and instruction

The Spectra and Dynamics of Diatomic Molecules

The topics covered in this book provide a qualitative and sometimes quantitative classic description of the wide-band 0-THz dielectric spectra of polar liquids, molecular libration-rotation (which is the reason for dielectric loss and absorption of electromagnetic waves), simple molecular models differing by the intermolecular-potential profiles, and present a comparison between the theoretical and experimental dependencies and derivation of the main results. A new feature is the application of a number of analytical models to different substances, including strongly absorbing nonassociating liquids, liquid water, water bound by macromolecules, and gas-like liquids. The presentation of the theory in this book is also new. It is based on the dynamic method in which the Brownian reorientations are considered implicitly, without direct solution of stochastic equations. This approach simplifies the theory. Senior students and experimentalists will find many of the results valuable.

Dynamics of Gas-Surface Interactions

This book provides fundamental knowledge in the fields of attosecond science and free electron lasers, based on the insight that the further development of both disciplines can greatly benefit from mutual exposure and interaction between the two communities. With respect to the interaction of high intensity lasers with matter, it covers ultrafast lasers, high-harmonic generation, attosecond pulse generation and characterization. Other chapters review strong-field physics, free electron lasers and experimental instrumentation. Written in an easy accessible style, the book is aimed at graduate and postgraduate students so as to support the scientific training of early stage researchers in this emerging field. Special emphasis is placed on the practical approach of building experiments, allowing young researchers to develop a wide range of scientific skills in order to accelerate the development of spectroscopic techniques and their implementation in scientific experiments. The editors are managers of a research network devoted to the education of young scientists, and this book idea is based on a summer school organized by the ATTOFEL network.

The Spectra and Dynamics of Diatomic Molecules

This book is written for graduate students just beginning research, for theorists curious about what experimentalists actually can and do measure, and for experimentalists bewildered by theory. It is a

guide for potential users of spectroscopic data, and uses language and concepts that bridge the frequency-and time-domain spectroscopic communities. Key topics, concepts, and techniques include: the assignment of simple spectra, basic experimental techniques, definition of Born-Oppenheimer and angular momentum basis sets and the associated spectroscopic energy level patterns (Hund's cases), construction of effective Hamiltonian matrices to represent both spectra and dynamics, terms neglected in the Born-Oppenheimer approximation (situations intermediate between Hund's cases, spectroscopic perturbations), nonlinear least squares fitting, calculation and interpretation of coupling terms, semi-classical (WKB) approximation, transition intensities and interference effects, direct photofragmentation (dissociation and ionization) and indirect photofragmentation (predissociation and autoionization) processes, visualization of intramolecular dynamics, quantum beats and wavepackets, treatment of decaying quasi-eigenstates using a complex Heff model, and concluding with some examples of polyatomic molecule dynamics. Students will discover that there is a fascinating world of cause-and-effect localized dynamics concealed beyond the reduction of spectra to archival molecular constants and the exact ab initio computation of molecular properties. Professional spectroscopists, kinetics, ab initio theorists will appreciate the practical, simplified-model, and rigorous theoretical approaches discussed in this book. Key Features: • A fundamental reference for all spectra of small, gas-phase molecules. • It is the most up-to-date and comprehensive book on the electronic

spectroscopy and dynamics of diatomic molecules. • The authors pioneered the development of many of the experimental methods, concepts, models, and computational schemes described in this book. A fundamental reference for all spectra of small, gas-phase molecules. It is the most up-to-date and comprehensive book on the electronic spectroscopy and dynamics of diatomic molecules. The authors pioneered the development of many of the experimental methods, concepts, models, and computational schemes described in this book.

Attosecond and XUV Physics

Proceedings of the NATO Advanced Research Workshop, held in Balatonföldvár, Hungary, 8-12 June 2003

Low-Energy Electron Scattering from Molecules, Biomolecules and Surfaces

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.

The Theory of Chemical Reaction Dynamics

Jet Spectroscopy and Molecular Dynamics

Advances in Theoretically Interesting Molecules: A Research Annual, Volume 2 provides information pertinent to the dynamics of cyclooctatetraene ring inversion. This book deals with bridgehead olefins, which helps to shed light on structure-activity relationships for this most basic functional group. Organized into four chapters, this volume begins with an overview of the involvement of planar, delocalized transition states to account for bond shifting in cyclooctatetraenes, which faces explicit problems in rationalizing the universally low energy demands. This text then examines the carbon-carbon double bond, which is the most ubiquitous functional group in organic chemistry. Other chapters consider the condensed polycyclic benzenoid aromatic hydrocarbons (PAHs), which is a subset of the multifarious class of polynuclear aromatics. This book discusses as well the problem of categorizing the molecular structures of PAHs. The final chapter deals with the reactions and synthesis of Dewar furan. This book is a valuable resource for organic chemists.

Proceedings of the International Conference of Computational Methods in Sciences and Engineering 2003 (ICCMSE 2003)

A comprehensive discussion of the key role of modern

spectroscopic investigations in interdisciplinary materials science and engineering, covering emerging materials that are either absolutely novel or well-known materials with recently discovered, exciting properties. The types of spectroscopy discussed include optical, electronic and magnetic, UV-visible absorption, Rayleigh scattering, photoluminescence, vibrational, magnetic resonance, electron energy loss, EXAFS, XANES, optical tomography, time-resolved spectroscopy, and point contact spectroscopy. The materials studied are highly topical, with a focus on carbon and silicon nanomaterials including nanotubes, fullerenes, nanoclusters, metallic superconducting phases, molecular materials, magnetic and charge-stripe oxides, and biomaterials. Theoretical treatments are presented of molecular vibrational dynamics, vibration-induced decay of electronic excited states, nanoscale spin-orbit coupling in 2D Si-based structures, and the growth of semiconductor clusters.

Numerical Hamiltonian Problems

Coherent Dynamics of Small Molecules in Rare Gas Crystals

This book is based on a NATO Advanced Study Institute held to enhance our understanding, at both an experimental and a theoretical level, of the molecular dynamics in liquid crystals. The lecturers at the Institute, each leaders in their respective fields, have contributed chapters to the book with the aim of

producing, for the first time, a coherent, pedagogical account of this interdisciplinary subject. The range of materials considered is wide, including lyotropic and thermotropic liquid crystals, biological membranes and polymeric systems. The formalism needed to characterise the rotational, translational and conformational dynamics is developed. Then the use of experimental techniques to investigate the dynamics is described; these techniques include NMR and ESR spectroscopy, neutron scattering, dielectric relaxation, infrared spectroscopy and fluorescence depolarisation. Some of these experiments are influenced by the collective orientations or director modes which are also considered. The results of these experiments are presented and the theory necessary to understand them is described, with particular attention being paid to the influence of the long range liquid--crystalline order on the dynamics.