

THEORETICAL STUDIES OF CHEMICAL DYNAMICS: Overview of Some Fundamental Mechanisms

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KEY WORDS: chemical reaction, nonadiabatic transition, superexcited state, multidimensional tunneling

ABSTRACT

Recent remarkable progress in theoretical studies of (*a*) quantum dynamics of chemical reactions, (*b*) characteristics and dynamics of superexcited states of molecules, (*c*) nonadiabatic transitions at potential curve crossings, and (*d*) multidimensional tunneling is reviewed briefly. Underlying common basic concepts and fundamental mechanisms such as adiabaticity and nonadiabatic transition are extracted and discussed in order to facilitate a comprehensive understanding of chemical dynamics. Not only the basic theoretical methodologies but also the intriguing dynamical aspects of each subject are explained as simply as possible.

Introduction

"Chemical dynamics" implies all kinds of dynamic phenomena in chemistry and is very multifarious, covering many spectroscopic processes, nonreactive collision processes, and chemical reactions (1). Chemical systems usually have strong personalities without any global symmetries and are composed of relatively large numbers of interrelated degrees of freedom. The mechanisms of their dynamic processes are diverse and do not seem to be systematized easily. To some extent, however, we can untangle the complicated processes and find some common basic features and mechanisms among them. The most basic mechanisms may be classified according to the characters of the states (electronic and rovibrational) that participate in the processes we are interested in. When the number of degrees of freedom increases, stochasticity comes into play, in addition to personality and selectivity.

Theoretical Chemical Dynamics Studies Of Reactions In Energetic Materials

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Theoretical Chemical Dynamics Studies Of Reactions In Energetic Materials:

Richtlinien für die Überwachung von Wehrmachtangehörigen ausserhalb der geschlossenen Truppe und von Betreuungseinrichtungen in den Niederlanden ,1942 **Chemical Dynamics Studies of Reactions in Energetic**

Materials ,1993 We have carried out a research program to investigate the chemical dynamics of unimolecular reactions in large polyatomic molecules The purpose of the studies is an improved understanding of the fundamental behavior of highly excited reactive molecules with an emphasis on energetic materials We have made some significant progress in extending theoretical chemical dynamics calculations to reactions in large molecules as illustrated by our explicit full dimensional classical dynamics study of the unimolecular decomposition of RDX Leading up to this study of RDX we performed a long series of dynamics calculations 2 30 for a variety of molecules to determine the important factors for accurately simulating processes in polyatomic molecules **Energetic Materials** ,2003-11-25 This volume provides an overview of current

research and recent advances in the area of energetic materials focusing on decomposition crystal and molecular properties The contents and format reflect the fact that theory experiment and computation are closely linked in this field Since chemical decomposition is of fundamental importance in energetic performance this volume begins with a survey of the decomposition processes of a variety of energetic compounds This is followed by detailed studies of certain compounds and specific mechanisms such as nitro aci nitro tautomerism Chapter 6 covers the transition from decomposition to crystal properties with molecular dynamics being the primary analytical tool The next several chapters deal with different aspects of the crystalline state again moving from the general to particular There is also a discussion of methods for computing gas liquid and solid phase heats of formation Finally the last portion of this volume looks at the potential of high nitrogen molecules as energetic systems this has been of considerable interest in recent years Overall this volume illustrates the progress that has been made in the field of energetic materials and some of the areas of current activity It also indicates the challenges involved in characterizing and understanding the properties and behaviour of these compounds The work is a unique state of the art treatment of the subject written by pre eminent researchers in the field Overall emphasis is on theory and computation presented in the context of relevant experimental work Presents a unique state of the art treatment of the subject Contributors are preeminent researchers in the field **Scientific and Technical Aerospace Reports** ,1995

AFOSR Chemical & Atmospheric Sciences Program Review United States. Air Force. Directorate of Chemical and Atmospheric Sciences, US Air Force Research Technology Area Plan ,1991 Advances in Chemical Reaction Dynamics Peter M. Rentzepis,Christos Capellos,2012-12-06 This book contains the formal lectures and contributed papers presented at the NATO Advanced Study Institute on the Advances in Chemical Reaction Dynamics The meeting convened at the city of Iraklion Crete Greece on 25 August 1985 and continued to 7 September 1985 The material presented describes the fundamental and recent advances in experimental and theoretical aspects of reaction dynamics A large section is devoted to

electronically excited states ionic species and free radicals relevant to chemical systems In addition recent advances in gas phase polymerization formation of clusters and energy release processes in energetic materials were presented Selected papers deal with topics such as the dynamics of electric field effects in low polar solutions high electric field perturbations and relaxation of dipole equilibria correlation in picosecond laser pulse scattering and applications to fast reaction dynamics Picosecond transient Raman spectroscopy which has been used for the elucidation of reaction dynamics and structural changes occurring during the course of ultrafast chemical reactions propagation of turbulent flames and detonations in gaseous energetic systems are also discussed in some detail In addition a large portion of the program was devoted to current experimental and theoretical studies of the structure of the transition state as inferred from product state distributions translational energy release in the photodissociation of aromatic molecules intramolecular and intramolecular dynamic processes

DA Pam , Department of the Army Pamphlet , Innovative Physical Chemistry Perspectives

Praveen Kaushik, 2025-02-20 Innovative Physical Chemistry Perspectives offers a refreshing take on traditional concepts in physical chemistry presenting them through innovative approaches modern applications and interdisciplinary insights Authored by experts this comprehensive volume explores fundamental principles and cutting edge research topics inviting readers to engage with the dynamic and evolving landscape of physical chemistry Each chapter delves into specific aspects providing in depth discussions theoretical foundations and practical examples From nanochemistry and biomolecular interactions to quantum mechanics and statistical mechanics we cover a wide range of topics highlighting the interconnectedness of various subfields and their relevance to real world phenomena Through clear explanations illustrative examples and thought provoking discussions Innovative Physical Chemistry Perspectives aims to inspire curiosity critical thinking and a deeper appreciation for the complexities of matter and energy at the molecular level Whether you're a student researcher or enthusiast in the field this book serves as a valuable resource for expanding your knowledge and understanding With its emphasis on modern perspectives interdisciplinary approaches and practical applications Innovative Physical Chemistry Perspectives is set to become an essential reference for anyone seeking to explore physical chemistry from new and exciting angles

Research Interests of the Air Force Office of Scientific Research , 1991

Energy and Water Development Appropriations for 1993: Department of Energy FY 1993 budget justifications United States. Congress. House. Committee on Appropriations. Subcommittee on Energy and Water Development, 1992

Overviews Of Recent Research On Energetic Materials Donald L Thompson, Robert W Shaw, Thomas B Brill, 2005-08-02 Few books cover experimental and theoretical methods to characterize decomposition combustion and detonation of energetic materials This volume by internationally known and major contributors to the field is unique because it summarizes the most important recent work what we know with confidence and what main areas remain to be investigated Most chapters comprise summaries of work spanning decades and contain expert commentary available nowhere else Although energetic materials

are its focus this book provides a guide to modern methods for investigations of condensed and gas phase reactions Although these energetic reactions are complex and difficult to study the work discussed here provides readers with a substantial understanding of the behavior of materials now in use and a predictive capability for the development of new materials based on target properties Assessment of the Physical Sciences Directorate at the Army Research Office National Academies of Sciences, Engineering, and Medicine, Division on Engineering and Physical Sciences, Laboratory Assessments Board, Army Research Laboratory Technical Assessment Board, Panel on Review of Extramural Basic Research at the Army Research Laboratory, 2020-07-17 This report summarizes the 2019 findings of the Panel on Review of Extramural Basic Research at the Army Research Laboratory which reviewed the programs at the Army Research Office's Physical Sciences Directorate

ERDA Energy Research Abstracts United States. Energy Research and Development Administration, 1976-05

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Energy and Water Development Appropriations for 1994 United States. Congress. House. Committee on Appropriations. Subcommittee on Energy and Water Development, 1993 **Toward Detonation Theory** Anatoly N. Dremin, 2012-12-06 It is known that the Chapman Jouguet theory of detonation is based on the assumption of an instantaneous and complete transformation of explosives into detonation products in the wave front Therefore one should not expect from the theory any interpretations of the detonation limits such as shock initiation of detonation and kinetic instability and propagation failure diameter The Zeldovich Von Neuman Doring ZND theory of detonation appeared in fact as a response to the need for a theory capable of interpreting such limits and the ZND detonation theory gave qualitative interpretations to the detonation limits These interpretations were based essentially on the theoretical notion that the mechanism of explosives transformation at detonation is a combustion of a layer of finite thickness of shock compressed explosive behind the wave shock front with

the velocity of the front. However, some experimental findings turned out to be inconsistent with the theory. A very small change of homogeneous liquid explosives detonation velocity with explosive charge diameter near the rather sizable failure diameter is one of the findings. The elucidation of the nature of this finding has led to the discovery of a new phenomenon. This phenomenon has come to be known as the breakdown (BD) of the explosive self-ignition behind the front of shock waves under the effect of rarefaction waves.

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