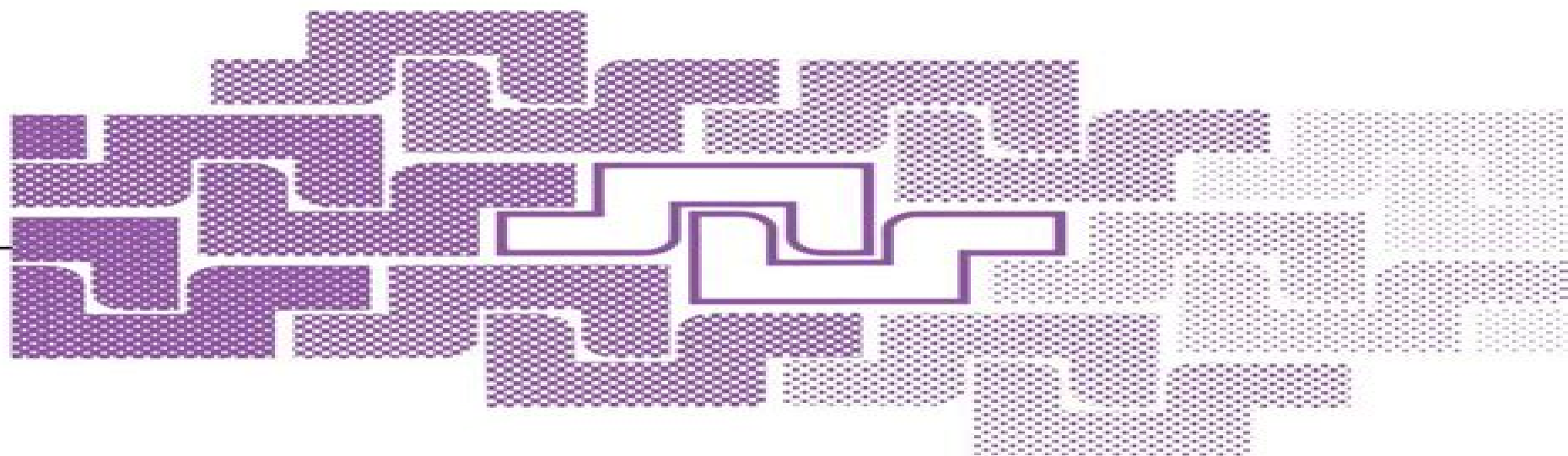




Stochasticity and Intramolecular Redistribution of Energy

edited by R. Lefebvre and S. Mukamel

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Stochasticity And Intramolecular Redistribution Of Energy

Antonio Laganà

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Stochasticity And Intramolecular Redistribution Of Energy:

Stochasticity and Intramolecular Redistribution of Energy Roland Lefebvre, S. Mukamel, 2012-12-06 This volume contains the invited papers presented at the NATO Advanced Research Workshop on Stochasticity and Intramolecular Redistribution of Energy held in Orsay France from June 23 to July 3 1986 The Workshop brought together leading researchers involved in the experimental and the theoretical studies of vibrational energy flow and relaxation in activated polyatomic molecules The recent experimental developments in this area include the study of ultracold molecules in supersonic beams and the development of high resolution frequency domain and ultrafast time domain spectroscopic techniques On the theoretical side the introduction of statistical methods random matrix theory reduced equations of motion and efficient numerical algorithms provide an adequate framework for the interpretation of vibrational dynamics in large polyatomic molecules Classical semiclassical and quantum calculations on simple model systems show the existence of regular and chaotic regions in the phase space The articles in this volume provide an updated review of the current status of experimental studies and the relevance of the recent theoretical developments to their interpretation We wish to thank the organizations which made this workshop possible NATO provided the basic grant We acknowledge the essential contribution of the late Dr Mario di Lullo in providing pertinent advice The generous support of the U S Air Force Office of Scientific Research the U S Advances in Multiphoton Processes and Spectroscopy S. H. Lin, A. A. Villaes, Y. Fujimura, 1993 In view of the rapid growth in both experimental and theoretical studies of multiphoton process and multiphoton spectroscopy of atoms ions and molecules in chemistry physics biology materials science etc it is desirable to publish an advanced series that contains review papers readable not only by active researchers in these areas but also by those who are not experts in the field but who intend to enter the field The present series attempts to serve this purpose Each review article is written in a self contained manner by the experts in the area so that the readers can grasp the knowledge in the area without too much preparation Soviet Journal of Chemical Physics ,1989 **Supercomputer Algorithms for Reactivity, Dynamics and Kinetics of Small Molecules** Antonio Laganà, 2012-12-06 The need for accurate computational procedures to evaluate detailed properties of gas phase chemical reactions is evident when one considers the wealth of information provided by laser molecular beam and fast How experiments By stressing ordinary scalar computers to their limiting performance quantum chemistry codes can already provide sufficiently accurate estimates of the stability of several small molecules and of the reactivity of a few elementary processes However the accurate characterization of a reactive process even for small systems is so demanding in terms of computer resources to make the use of supercomputers having vector and parallel features unavoidable Sometimes to take full advantage from these features all is needed is a restructure of those parts of the computer code which perform vector and matrix manipulations and a parallel execution of its independent tasks More often a deeper restructure has to be carried out This may involve the problem of choosing a suitable computational strategy or the

more radical alternative of changing the theoretical treatment There are cases in fact where theoretical approaches found to be inefficient on a scalar computer exhibit their full computational strength on a supercomputer Physics Briefs ,1992

AFOSR Chemical & Atmospheric Sciences Program Review United States. Air Force. Directorate of Chemical and Atmospheric Sciences, Large Finite Systems Joshua Jortner,A. Pullman,2012-12-06 The Twentieth 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 Twentieth Jerusalem Symposium marked an auspicious occasion commemorating two decades of this scientific endeavour The topic at this year s Jerusalem Symposium was Large Finite Systems which constitutes a truly interdisciplinary subject of central interest in the broad areas of chemistry physics astrophysics and biophysics The main theme of the Symposium was built around bridging the gap between molecular surface and condensed matter chemical physics Emphasis was placed on the interrelationship between the properties of large molecules van der Waals complexes and clusters focusing on the structure dynamics of nuclear motion quantum and thermodynamics size effects the nature of electronic states and excited state energetics and dynamics of large finite systems The interdisciplinary nature of these research areas was deliberated by intensive and extensive interactions between scientists from different disciplines and between theory and experiment This volume provides a record of the invited lectures at the Symposium **Photoselective Chemistry, Volume 47, Part 1** Joshua Jortner,2009-09-08 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 **Advances in Chemical Physics** Ilya Prigogine,Stuart Alan Rice,1958 **New Technical Books** New York Public Library,1988

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