Dynamics and Spectroscopy of Complex Molecular Systems

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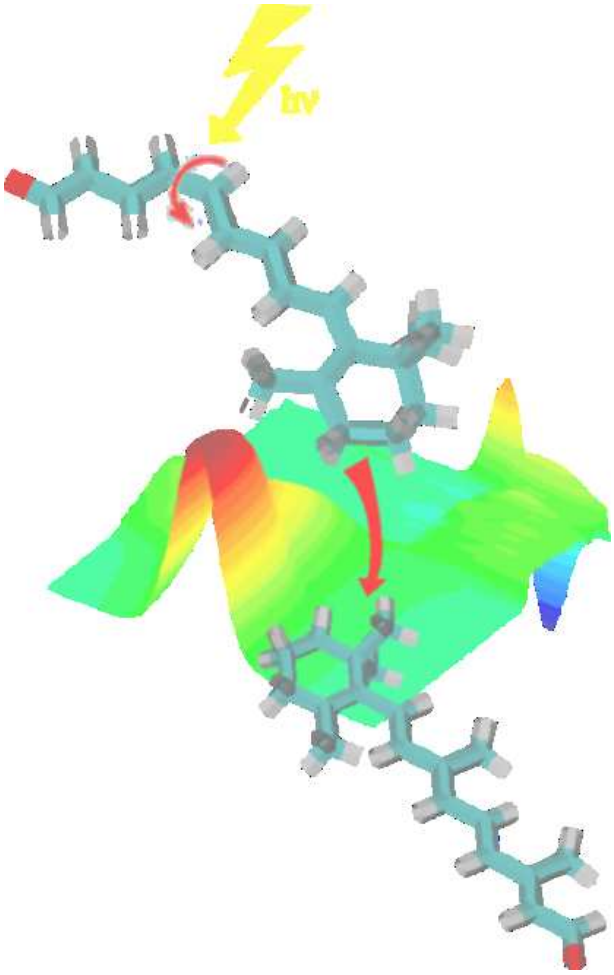

Preface

With the advent of femtosecond laser technology it has become possible to observe the dynamics of elementary molecular processes in *real time*. Following Zewail's pioneering experiments on simple gas-phase chemical reactions [1], numerous groups have revealed intriguing and so far unknown dynamic phenomena in more and more complex systems. For example, ultrafast photoreactions in proteins such as rhodopsin [2] (responsible for the vision in your eye) and highly efficient energy transfer processes in light harvesting systems [3] (responsible for photosynthesis) have shown that coherent quantum dynamics is even found in large biological systems. The wealth of experimental information has also made clear that time-dependent spectroscopy of complex molecular processes in general strongly depends on theoretical support. This has prompted a continuous development of powerful theoretical and computational methods that allow us to calculate dynamics and spectra from "*first principles*," i.e., from a quantum-mechanical or classical formulation independent from experimental input.

This course on *Dynamics and Spectroscopy* is aimed to introduce the main theoretical concepts of this field to graduate students of Physics and Chemistry. Although the manuscript is self-contained and aims to lead from simple to more involved physical problems, it can certainly not replace a good textbook on these matters. Time-dependent quantum mechanics and some spectroscopy is covered in the recent book by Tannor [4] and in the inexpensive textbook of Schatz and Ratner [5]. A readable book on relaxation theory was compiled by May and Kühn [6] and the "bible" on nonlinear spectroscopy was delivered by Mukamel [7].

I thank all the students who over the years helped to improve the manuscript by asking questions and making suggestions. I also thank Peter Hamm and Michael Thoss for many inspiring discussion and for numerous figures, slides, and other help they provided. Moritz Otten and Lukas Bruder helped to get the manuscript typed and illustrated. As it is still far from perfect, please mail corrections and comments to stock@physik.uni-freiburg.de.

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Contents

Spectroscopy and dynamics of bioanalytical, biomedical, environmental, and atmospheric sciences, Novel experimental techniques or instrumentation for molecular spectroscopy, Novel theoretical and computational methods, Novel applications in photochemistry and photobiology, Novel interpretational approaches as well as advances in data analysis based on electronic or vibrational spectroscopy.Â ZnCdO2 monolayer â€" A complex 2D structure of ZnO and CdO monolayers for photocatalytic water splitting driven by visible-light. Ze-Cheng Zhao | Chuan-Lu Yang | Metal ions-triggered photo-induced fluorescence change in rhodamine B-based photo-responsive complexes. Yuanyuan Li | Zining Feng | Molecular spectroscopy is a subject of quantum physics. Excitation of molecular movement or vibration as used with infrared (IR) spectroscopy or the excitation of an electron in a higher Ï€-orbital as used for ultraviolet/visible (UV/VIS) spectroscopy is possible in a normal surrounding. The excitation, in principle, requires two different energy levels: for IR and UV spectroscopy, respectively, these conditions are given at any place without the need of technical resources. However, this is not the case in NMR spectroscopy. The irradiated energy can only interact with the nuclear spin quantum complex molecular systems, either in the gas phase or in the condensed phase, taking examples from the infrared spectroscopy of N-methylacetamide and small peptides. Band assignments for the simulation is still challenging and we introduce here a general method for obtaining effective normal modes of molecular systems from Molecular Dynamics simulations. The effective normal modes are defined as linear combination of internal coordinates such that the power spectra of these modes are as localized as possible in frequency.Â 4 September, 0 : article Page of 0 environments and situations, while providing a description of the structure and dynamics of a system in its fluctuating environment at finite temperature.