
Preface

Molecular quantum dynamics is an emerging field at the border between quantum physics and chemistry. There is growing evidence that a significant number of chemical reactions are impacted by strong quantum-mechanical effects and, even more importantly, that these quantum effects, such as quantum coherence, could be used to create radically new technologies involving molecular systems. For instance, since the invention of lasers, it has become a dream in chemistry to use these coherent sources for triggering photochemical reactions selectively and efficiently. In traditional industrial chemistry, this is achieved by adjusting external parameters such as temperature, pressure, concentration, and solvent, or by adding catalysts. In general, much energy is wasted and many undesired by-products are created, which may have negative effects on the environment. In this context, laser light offers the possibility to deposit energy in a molecule and to trigger chemical reactions in a fully controlled fashion and in a much cleaner and energetically efficient way.

Since the advent of femtochemistry, the possibility to manipulate chemical reactivity by excitation with laser pulses has already been experimentally demonstrated for several reactions in the gas phase and on surfaces. For instance, the excitation of the stretching modes of vibration of CH_4 accelerates the C–H bond breaking on a surface of Ni(100). But a precise control of quantum effects in molecular processes still remains challenging due to the large number of vibrational and rotational degrees of freedom that can rapidly dissipate the quantum coherence. However, major experimental developments have been achieved recently: the possibility to align and even orientate molecules in two or three dimensions and attospectroscopy that allows one to generate sub-femtosecond laser pulses for observing electrons on their natural time scale. The conjunction of femto- and atto-chemistry and of the alignment of molecules lets us hope that it will be possible to reach a much higher level of control of chemical reactivity at its most fundamental level including the quantum effects that govern the microscopic realm.

In addition, during the last 20 years, tremendous progress has been made in the development and applications of theoretical approaches to the full quantum-mechanical study of molecular processes. This development has been made possible by the availability of powerful workstations and massively parallel computers and even more importantly by the design of new and more efficient algorithms to solve the Schrödinger equation. Perhaps the most significant result of this is that full quantum-mechanical simulations have allowed the correct interpretation

of major experimental findings. This is the aim of the present book, written by theoreticians, to provide some illustrations in a wide range of areas: heterogeneous catalysis, reactive scattering, photodissociation, infrared or ultraviolet spectroscopy, photochemistry guided by laser pulses, and quantum computing.

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