Quantum optimal control of molecular processes

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Over the past few years quantum control has proven to be very successful in steering molecular processes with modulated light fields. By combining theory and experiment, even highly complex control aims were realized, mostly in the gas phase. In the first part of the lecture, the basic concept of coherent control is introduced, sketching the way from single parameter to the multi parameter control in the time domain. Optimal control theory as one prominent representative of multi parameter control will be discussed in detail. As molecular systems offer a large variety of controllable degrees of freedom, the focus is on molecular reactions. These examples include the motion of the nuclei occurring on a time scale from femtoseconds to picoseconds and longer and require the solution of the time-dependent Schrödinger equation for the nuclear motion. Advancing control further to the domain of electron motion requires sub-femtosecond temporal resolution. This topic will be addressed in the second part of the lecture. Two strategies will be highlighted: (1) Control of electron dynamics via the carrier envelope phase in few cycle pulses and (2) via the temporal phase of a femtosecond laser pulse with attosecond precision. In this context the issue of nuclear and electronic wavepacket synchronization to achieve control on a chemical reaction is raised. A next step for the quantum control of chemical processes is to move on from isolated systems to systems in an environment, which can be e.g. a solution, a biological environment or a surface. For theory, this implies to include solvent effects in the quantum control simulations. In part three of this lecture two major concepts will be presented, namely an implicit description of the environment via the density matrix algorithm and an explicit inclusion of solvent molecules. All three parts of the course will be illustrated by examples from theory and experiment.

<u>Prerequisites for attending the lecture:</u> The lecture course is directed at students with a background in quantum mechanics and basic knowledge in molecular physics and spectroscopy.