Electron dynamics and its control in molecules
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The accessibility of few femtosecond or even attoseconds pulses opens the door to direct observation of electron dynamics. The idea to steer chemical reactions by localization of electronic wavepackets is intriguing, since electrons are directly involved in bond breaking and formation. The formation of a localized electronic wavepacket requires the superposition of two or more appropriate electronic states. Its guidance is only possible within the coherence time of the system and has to be synchronized with the vibrational molecular motions. In theoretical studies we elucidate the role of electron wavepacket motion for the control of molecular processes. We give three examples with direct connection to experiments. From our analysis, we extract the systems requirements defining the time window for intramolecular electronic coherence, the basis for efficient control. Based on these findings we map out a photoreaction that allows direct control by guiding electronic wavepackets. The carrier envelope of a femtosecond few cycle IR pulse is the control parameter that steers the photoreaction through a conical intersection.

References: