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Attosecond Molecular Dynamics

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The development of attosecond laser pulses allows one to probe the inner working of atoms, molecules and surfaces on the timescale of the electronic response. In molecules, attosecond pump-probe spectroscopy enables investigations of the prompt charge redistribution and localization that accompany photo-excitation processes, where a molecule is lifted from the ground Born-Oppenheimer potential energy surface to one or more excited surfaces, and where subsequent photochemistry evolves on femto- and attosecond timescales. In this talk I will present a few theoretical examples of realistic molecular attosecond pump-probe experiments in which simple molecules are ionized with a single attosecond pulse (or a train of attosecond pulses) and are subsequently probed by one or several infrared or xuv few-cycle pulses. The evolution of the electronic and nuclear densities in the photo-excited molecule or remaining molecular ions is calculated with attosecond time-resolution and is visualized by varying the delay between the pump and probe pulses. The results of these calculations [1-7] allow us to explain several experimental observations as well as to guide future experimental efforts to uncover ultrafast electron and nuclear dynamics in molecules.

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