Control of high-field phenomena on molecules and clusters: ionization and high harmonic generation.

A. Castro[1], E. Räsänen[1], A. Akbari[2], A. Rubio[2] and E. K. U. Gross[1]

[1] *Institut für Theoretische Physik, Fachbereich Physik der Freie Universität Berlin, Germany*

[2] *Departamento de Física de Materiales, Facultad de Ciencias Químicas, UPV/EHU, Centro Mixto CSIC-UPV/EHU and Donostia International Physics Center, San Sebastián, España*

alberto@physik.fu-berlin.de

When irradiated with high-intensity electromagnetic pulses, clusters and molecules react in complex manners. Multi-photon, tunneling and over-the-barrier ionization, laser driven photo-induced isomerizations or fragmentations, and high harmonic generation are some of the non-linear effects that are observed. We employ time-dependent density-functional theory (TDDFT) to study these processes and, in a further step, we couple TDDFT to the techniques of quantum optimal control theory (QOCT) in order to predict, computationally, those external fields that enhance a given desired effect. We provide two examples: femtosecond laser pulse shaping for enhanced ionization, and for optimizinig the high harmonic yield.

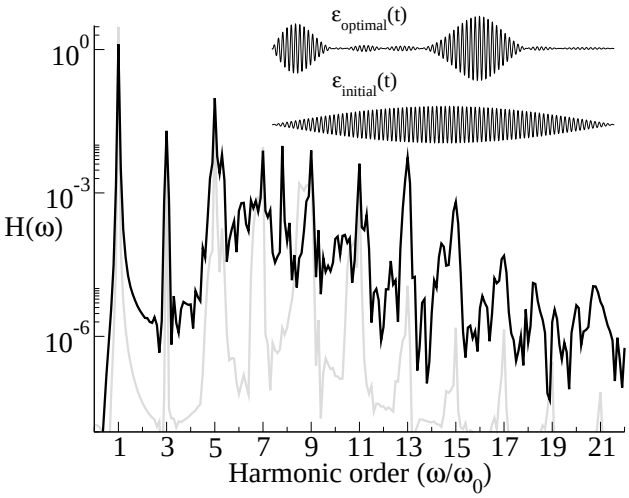

Figure 1: Harmonic spectra emittted by a Hydrogen molecule: In grey, the spectrum generated by an initial cosine-shaped pulse of approx. 170 fs; in black, the spectrum generated by the optimized laser pulse: an enhancement of the intensity of the higher harmonics can clearly be observed.