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Study of attosecond dynamics of small and medium sized molecules induced by ultra-short optical pulses using TD-DFT MICAEL OLIVEIRA, GABRIELE D'AVINO, Département de Physique, Université de Liège, Belgium, TOMASZ KUS, BENOIT MIGNOLET, Département de Chimie, Université de Liège, Belgium, THEODOROS PAPADOPOULOS, Institute of Renewable Energy and Environmental Technologies (IREET), Department of Engineering, Bolton, UK, FRANÇOISE REMACLE, Département de Chimie, Université de Liège, Belgium, MATTHIEU VERSTRAETE, Département de Physique, Université de Liège, Belgium — The advent of attosecond optical pulses, by allowing to control the breaking and rearrangement of chemical bonds, opens the door to many new applications, like novel catalysis mechanisms, photosensitive reactions, the preparation of states for quantum computing, etc. This control of the chemistry is made possible by the time scale of the attosecond pulses, which are effectively instantaneous with respect to the movement of the atomic nuclei, thus allowing the generation of a population of electronic states which is strongly out of equilibrium. In this work we investigate the electron dynamics of several molecular systems under the influence of attosecond pulses using the real-time formulation of time-dependent density functional theory (TD-DFT). We show a comparison of the performance of several exchange-correlation functionals by comparing TD-DFT calculations with equation of motion CCSD and CAS-SCF quantum chemistry methods, as well as applications of the method to the simulation of transient absorption spectroscopy.

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