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Ultrafast Coherent Electronic and Nuclear Dynamics Induced by Attopulses

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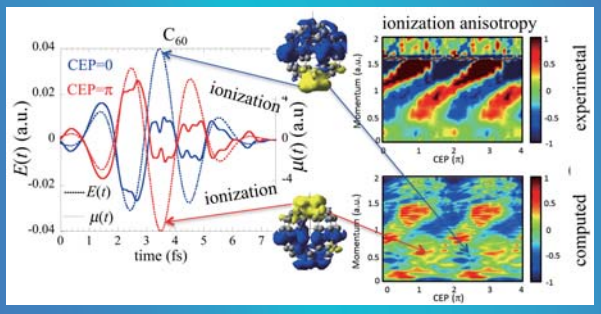
Since the recent developments in the generation of optical attopulses it is becoming experimentally feasible to induce and subsequently directly probe ultrafast charge transfer in modular molecules. One ultrafast pulse creates a non-stationary state of the neutral or of the cation that can be probed by a second pulse. Such experiments allow characterizing a purely electronic time scale, before the coupling to the nuclei takes place.[1] We are now investigating how the onset of nuclear motion and subsequently the fate of a chemical reaction can be controlled by tailoring this non equilibrium electronic density through a strong ultra short excitation pulse.
I will report on the simulation of realistic pump-probe experiments that monitor the ultrafast non equilibrium electronic dynamics including the ionization continua and field effects in LiH,[2] in the bifunctional molecule $C_{10}H_{15}N$ [3], in C_{60}[4] and in ICCH.[5] I will then discuss the role of nuclear motion in LiH[6] and in HCN[7] using full electron–nuclei quantum dynamics computation. These computations show that the ultrafast beatings of the electronic coherences in space and in time are modulated by the different periods of the nuclear motion but survive for a large number of vibrational periods. Our results also show that dissociation to specific asymptotes can be controlled through the CEP phase of an essentially one cycle IR pulse.



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[6] A. Nikodem, R. D. Levine, F. Remacle, *Phys. Rev. A* 2017, **95**, 053404.
[7] S. van den Wildenberg, B. Mignolet, R. D. Levine,F. Remacle, *PCCP* 2017, **19**, 19837 - 19846.

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