SEMINAIRE ISMO

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Ab-initio simulations of ultrafast electronuclear dynamics : paving the way to attochemistry

The advent of attosecond physics allowed the observation and manipulation of dynamic processes occurring within the intrinsic time scale of charge motion at atomic scale. This has opened the door to the realization of the dream of attochemistry, namely to control chemical reactions through the manipulation of the pure electronic dynamics taking place in the first instants after the excitation of the system. The full simulation of such a control scheme is a multi-scale problem going from the initial ionization triggering the dynamics to the final chemical reaction of the molecule.

In this seminar, I will present results exemplifying different aspects of attochemistry, paving the way to its full simulation. I will talk about pure electron dynamics triggered by ionization, termed charge migration, and how it is possible to control the charge migration process with tailored IR pulses. Using the propiolic acid molecule, for which we had performed a fully quantum treatment of the electronuclear dynamics, it will be shown that even though the nuclear motion can lead to a very fast decoherence of the electron dynamics, long lived electron coherences are possible. Using the same formalism, I will also present results on XUV induced non-adiabatic dynamics of PAHs in the context of astrochemistry. Finally, dipole induced sub-cycle modulation of the ionization rate will be discussed.

Mardi 17 septembre 2019 à 11 h

Amphithéâtre du bât 520 (3ème étage)

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