

SEMINAIRE ISMO

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Ultrafast electron dynamics as a route to explore chemical processes

Exposing molecules to ultrashort laser pulses can trigger pure electron dynamics in the excited or ionized system. In the case of ionization, these dynamics may manifest as an ultrafast migration of the initially created hole-charge throughout the ionized molecule and were termed charge migration. Charge migration can be solely driven by electron correlation and appeared to be a rich phenomenon with many facets that are rather characteristic of the molecule studied. Importantly, due to the coupling between the electronic and the nuclear motion, the control over the pure electron dynamics offers the extremely interesting possibility to steer the succeeding chemical reactivity by predetermining the reaction outcome at a very early stage. This is the paradigm of the emerging field of “attochemistry”. It will be shown how by appropriately tailored ultrashort laser pulses one can control the ultrafast charge migration in experimentally interesting molecules. Full quantum electron-nuclear dynamics calculations of the charge dynamics initiated by ionization will be presented and the possibilities to realize the dream of attochemistry, namely achieving control of chemical reactions by manipulation of electron coherences, will be discussed.

Mardi 14 mai 2019 à 11 h

Amphithéâtre du bât 520 (3^{ème} étage)

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