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SEMINAIRE LIDYL

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- Bâtiment 522 - Salle 138

“Ultrafast molecular dynamics induced by XUV attosecond pulses”

Attosecond science is nowadays a well-established research field, which offers formidable tools for the investigation and control of electronic processes [1]. In the last few years, attosecond pulses have been used to measure the ultrafast electron dynamics occurring in atoms, small molecules and solids. Electron dynamics plays a very important role in bond-formation and bond-breakage, thus determining the final chemical reactivity of a molecule. Recently, theoretical studies have pointed out that after sudden ionization of a large molecule very efficient charge migration, driven by purely electronic effects, can occur on a temporal scale ranging from few femtoseconds down to tens of attoseconds [2].

In this talk I will first show that XUV attosecond pulses in combination with NIR/VIS few-cycle pulses can be used to investigate charge migration in aromatic amino acids. By measuring the time evolution of the yield of the doubly charged immonium ion for phenylalanine and tryptophan we were able to identify the presence of fast modulations of the dication yield with periodicities of 4.3 fs for phenylalanine and 3.9 fs for tryptophan. This fast dynamics has been assigned to electronic beatings occurring between different functional groups of the molecule [4,5].

I will then show that the same time-resolved measurement can be exploited to measure in real-time hydrogen migration occurring in 5-halo-uracils such as 5FU and 5BrU. In the case of 5FU, the XUV pulse ionizes the molecule catalyzing the hydrogen migration from C6 to C5 at the first step of the reaction, leading to the fragment $m/z=44$. The pump-probe measurement reveals that at early times, the NIR-VIS pulse inhibits the hydrogen migration process thus resulting in a sudden reduction of fragments $m/z=44$, and a consequent increase of fragment $m/z=43$. The rising (decaying) dynamics associated to fragment $m/z=44$ ($m/z=43$) occurs with a time constant of about 35 fs which can be associated to the time required by the hydrogen atom to migrate from the C6 site to the C5 site of the molecule. Similar behaviors were observed for the equivalent 5BrU fragments.

Finally, a recent time-resolved study of photo-fragmentation of the nucleobase adenine, a molecule of key biological importance, will be presented. The most intriguing observation is that a stable dication of the parent molecule can be produced if (and only if) the probing NIR pulse is very briefly delayed from the XUV pulse. The delayed formation of the parent dication suggests the presence of a non-adiabatic relaxation mechanism occurring in the highly excited cationic states.

[1] P. B. Corkum & F. Krausz, *Nature Physics* 3, 381-387 (2007)

[2] L. S. Cederbaum et al *Chem. Phys. Lett.* 307, 205 (1999)

[3] F. Calegari et al., *Science* 346, 336 (2014)

[4] F. Calegari et al., *IEEE JSTQE* 21, 2419218 (2015)

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