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Séminaire du LCPMR

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Photo-induced ultrafast nuclear dynamics in core-excited molecules

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In the seminar I will discuss selected achievements of my previous works obtained during my postdoctoral and Marie-Curie fellowships at the synchrotron radiation facility SOLEIL and I will describe the first results of the current projects in which I am involved since October 2014 at the Laboratoire de Chimie Physique-Matière et Rayonnement (LCPMR) in the group of Marc Simon.

My previous research was focused on soft X-ray synchrotron radiation-based spectroscopic studies of electronic structure and ultrafast relaxation dynamics of neutral core-excited ($core^{-1}V$) molecules, where the core hole is short-lived (3-8 fs). Resonant Auger spectroscopy (RAS) was the main investigation tool in the studies of femtosecond nuclear dynamics. In particular, a new mechanism of ultrafast dissociation was discovered for molecules yielding heavy fragments after dissociation within only few femtoseconds owing to the internal motion of light linkages [1]. It was demonstrated that the state-of-the-art RAS can be used to 'image' potential-energy curves by controlling the X-ray-driven nuclear wave packet in the core-excited state [2]. Einstein-Bohr gedanken experiment was performed at the molecular level and continues one of the richest public debates in the history of Science on wave-particle duality [3]. Additionally, a high-resolution valence photoionization experiment will be described, which enables to trace the ejected photoelectrons back to their atom of origin [4].

The current projects deal with hard X-ray (>1 keV) photoelectron spectroscopies. Hard X-ray photons may reach deeper-lying core electrons. The lifetime (τ) of deep-core-hole states is very short – of the order of 1 fs or below, which does not allow for extensive nuclear dynamics to take place before electronic relaxation occurs. However, creation of deep core holes may lead to dissociation on a few-femtosecond timescale despite the very short (≤1 fs) lifetime of such states. This is because the 1st steps of the relaxation processes (i.e. both radiative and non-radiative decays) generate intermediate states with one and multiple holes in core orbitals. As an example, ultrafast dissociation is observed after Cl 1s→σ* in every step of the LVV *Auger* decay channels in HCl before the next electronic relaxation takes place.

REFERENCES

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[2] C. Miron *et al.* Nature Physics **8**, 135 (2012).
[3] X.-J. Liu *et al.*, Nature Photonics **9**, 120 (2015).
[4] C. Miron *et al.* Nature Communications **5**, 3816 (2014).