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## Photo-induced ultrafast dissociation following deep-core-electron excitation

Oksana Travnikova<sup>\*◇1</sup>, Tatiana Marchenko<sup>\*◇</sup>, Gildas Goldsztejn<sup>\*◇</sup>, Renaud Guillemin<sup>\*◇</sup>,  
Loïc Journal<sup>\*◇</sup>, Denis Céolin<sup>‡</sup>, Kari Jänkälä<sup>∇</sup>, Ralph Püttner<sup>†</sup>, Hiroshi Iwayama<sup>∪</sup>, Eiji  
Shigemasa<sup>∪</sup>, Stéphane Carniato<sup>\*◇</sup>, Maria Novella Piancastelli<sup>\*◇∧</sup> and Marc Simon<sup>\*◇‡</sup>

\* CNRS, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75005 Paris, France

◇ Sorbonne Universités, UPMC Univ Paris 06, UMR 7614, Laboratoire de Chimie Physique-Matière et Rayonnement, F-75005 Paris, France.

∇ Department of Physics, University of Oulu, P. O. Box 3000, 90014 Oulu, Finland

† Institut für Experimentalphysik, Freie Universität Berlin, D-14195 Berlin, Germany

‡ Synchrotron SOLEIL, l'Orme des Merisiers, Saint-Aubin, F-91192 Gif-sur-Yvette Cedex, France

∧ Department of Physics and Astronomy, Uppsala University, SE-75120 Uppsala, Sweden

∪ Ultraviolet Synchrotron Orbital Radiation Facility, Institute for Molecular Science, Okazaki 444-8585, Japan

**Synopsis** Creation of deep core holes leads to extensive nuclear dynamics on a few femtosecond timescale despite the very short ( $\tau \leq 1$  fs) lifetime of such states. This is because the 1<sup>st</sup> 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 in three well-distinguishable LVV Auger decay channels for HCl following Cl1s $\rightarrow\sigma^*$  excitation.

Absorption of an X-ray photon by a molecule may lead to the excitation of a localised core electron to a specific unoccupied valence orbital if the energy of the photon matches exactly the difference between the involved core and valence electronic levels. The created core-hole states are highly unstable and eventually decay on a very short timescale emitting a photon (radiative decay) or a so-called Auger electron (non-radiative or Auger decay).

Hard X-ray photons ( $>1$ keV) may reach deeper-lying core electrons. The lifetime ( $\tau$ ) of deep-core-hole states is very short – of the order of 1 fs or below. Nevertheless, the signature of nuclear dynamics was observed for Cl1s $\rightarrow\sigma^*$  ( $\tau \approx 1$  fs) core-excited states of HCl [1] and even on a sub-femtosecond timescale ( $\tau \approx 200$  attoseconds) in the case of I2p $\rightarrow 15a_1^2$  core electron transitions in CH<sub>3</sub>I [2].

The electronic relaxation dynamics of deep-core-hole states is very rich. At variance with that, the very short lifetimes of these states do not allow for extensive nuclear dynamics to take place before electronic relaxation occurs. However, the dominant channels of the 1<sup>st</sup> step relaxation processes (both radiative and Auger decays) lead to intermediate states which bear 1 or 2 holes in core-electron shells. In the HCl molecule, the leading relaxation decays of the Cl1s $^{-1}\sigma^*$  state are Auger KLL and radiative K $\alpha$  channels, which create Cl2p $^{-2}\sigma^*$  and Cl2p $^{-1}\sigma^*$  intermediate states, respectively. The latter one can be created by direct soft X-ray absorption

and has been well characterised [3]. It is known to undergo ultrafast dissociation (UFD) within the Cl2p $^{-1}$  lifetime of  $\sim 8$  fs [3, 4]. The former double core-hole Cl2p $^{-2}\sigma^*$  states are yet exotic and can be also created as so-called “super”-satellites [5] of direct 2p $^{-2}$  double core-hole ionisation. Very recent theoretical studies [5] show that the energy gradients of the core $^{-2}$ V states can be very large (3 times larger compared to the core $^{-1}$ V state in the case of H<sub>2</sub>O [5]). Therefore, nuclear dynamics is correspondingly faster in core $^{-2}$ V “super”-satellites.

Our experimental measurements reveal UFD phenomena in Cl2p $^{-2}\sigma^*$  state of HCl with  $\tau$  only about 3 fs. The measured LVV Auger decay spectrum of HCl clearly shows 3 possible decay channels following Cl1s $\rightarrow\sigma^*$  excitation. In fact, ultrafast dissociation is observed in *every* step of these LVV decay channels before the next electronic relaxation takes place. The observed results are supported by *ab initio* theoretical calculations.

### References

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<sup>1</sup>E-mail: oksana.travnikova@upmc.fr

