

# High Resolution Spectroscopies of Isolated Species: present and future directions

*In honor of the 80<sup>th</sup> birthday of Professor T. Darrah Thomas*

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# Double Core-hole Spectroscopy Experimental Aspects

F. Penent<sup>1</sup>, P. Lablanquie<sup>1</sup>, J. Palaudoux<sup>1</sup>, L. Andric<sup>1</sup>, P. Selles<sup>1</sup>,  
S. Carniato<sup>1</sup>, M. Žitnik<sup>2</sup>, T.P. Grozdanov<sup>3</sup>, E. Shigemasa<sup>4</sup>, K. Soejima<sup>5</sup>,  
Y. Hikosaka<sup>5</sup>, I. H. Suzuki<sup>6</sup>, M. Nakano<sup>6</sup> and K. Ito<sup>6</sup>

<sup>1</sup> LCP-MR, CNRS & Université P. VI, 11 rue P. et M. Curie, 75231 Paris Cedex 05, France

<sup>2</sup> Jožef Stefan Institute, P. O. Box 3000, SI-1001 Ljubljana

<sup>3</sup> Institute of Physics, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia

<sup>4</sup> UVSOR Facility, Institute for Molecular Science, Okazaki 444-8585, Japan

<sup>5</sup> Department of Environmental Science, Niigata University, Niigata 950-2181, Japan

<sup>6</sup> Photon Factory, Institute of Materials Structure Science, Oho, Tsukuba 305-0801, Japan

## ABSTRACT

Although the interest of molecular double core hole states (DCHs) for ESCA (Electron Spectroscopy for Chemical Analysis) was pointed out 25 years ago [1], their observation has been possible only very recently, thanks to the development of two different approaches: two-photon double-core ionization using XFEL sources [2] or single photon double-core ionization using synchrotron sources [3,4]. We have demonstrated that the latter method provides detailed information on the spectroscopy and decay dynamics of DCHs, even if the associated double photoionization cross section is extremely weak. We have observed single-site DCHs, (ss-DCHs:  $K^{-2}$ ) where the two core holes are created on the same atom of the molecule [3], and also two-site DCHs, (ts-DCHs:  $K^{-1}K^{-1}$ ), where the two core holes are on different atoms [4].

The experiments were performed at Photon Factory (Japan) and at SOLEIL (France), during single-bunch operation, using a magnetic bottle time-of-flight spectrometer. We have studied simple molecules:  $N_2$ ,  $O_2$ ,  $CO$ ,  $CO_2$  and  $C_2H_{2n}$  ( $n = 1, 2, 3$ ).

By detecting in coincidence two photoelectrons with one or two Auger electrons, we have characterized  $K^{-2}$  and  $K^{-1}K^{-1}$  states: their binding energies, their respective Auger decay paths and their relative intensity with respect to  $K^{-1}$  single ionization. Single photon double ionization leading to  $K^{-2}$  states represents a  $\sim 10^{-3}$  fraction of single K-shell ionization, this figure drops to  $\sim 10^{-5}$  for  $K^{-1}K^{-1}$  states formation. A simple collisional knock-out model, where an initially ionized K-shell electron hits and ejects a second K-shell electron from the neighboring atom accounts for this ratio.

These experimental results are important to understand the formation of DCHs by single photon absorption. The spectroscopy and the decay mechanisms of these highly excited species are obtained with high accuracy.

We will present at the workshop our most recent results on photon double K-shell ionization.

## REFERENCES

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