Core Ionization with Core Excitation: A New Spectroscopic Tool

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In the last few years, double core hole or K^{-2} states (DCHs) have been studied by single photon double core ionization on synchrotron centers [1] and by multiple photon ionization [2] on X-ray free electron lasers (XFELs).

Closely related to double core ionization, the single photon process where a core electron is ionized while another core electron is excited simultaneously has been observed. This $K^{-2}V$ spectroscopy provides a new insight on double core-hole states that combines the characters of both XPS and near-edge X-ray absorption fine structures (NEXAFS) spectroscopy.

As shown recently [3-7], theoretical investigations revealed interesting properties on the formation mechanisms of $K^{-2}V$ states. Studies of the C_2H_{2n} (n=1–3) series [3], N_2 [4], H_2O [5] and more recently on centrosymmetric CO_2 [6] molecule and Neon atom [7] demonstrated that two competing channels appear with comparable intensities. The first one corresponds to the dipolar ionization of a core electron accompanied by monopolar excitation (direct shake-up) of the remaining core electron. The second one corresponds to the dipolar excitation of a core electron to a vacant orbital accompanied by monopolar shake-off of the other core electron (conjugate shake-up process). This second process has a NEXAFS-like character.

After a brief presentation of the various specificities of $K^{-2}V$ vs $K^{-1}V$(NEXAFS)/ K^{-1}(XPS) spectroscopies, perspectives on what can FERMI free electron laser light source achieve for the study of $K^{-2}/K^{-2}V$ processes in complement to synchrotron radiation sources will be discussed.

References

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