Theoretical approaches for x-ray pump/x-ray probe spectroscopy

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Resolving the real-time motion of electrons in complex systems is key for enhancing the functionality and the understanding of the underlying mechanisms of relevant photo-induced processes. The advent of novel x-ray pump/x-ray probe capabilities at free electron lasers open the route to unprecedented applications in complex systems, in which an specific atomic site can be excited and, only few femtoseconds after, the induced dynamics can be probed in another site of the same system [1].

In order to retrieve information from these state-of-the-art experiments, novel theoretical developments that combine both inner-shell and valence dynamics are required. In this talk we will present some theoretical results for obtaining information of chemical environment changes in molecular systems with few-femtosecond resolution via time-resolved x-ray photoelectron spectroscopy (tr-XPS). We will also discuss the possibility to use tr-XPS for observing "in real time" hydrogen migration processes and Auger-induced charge migration [2], see Fig 1.

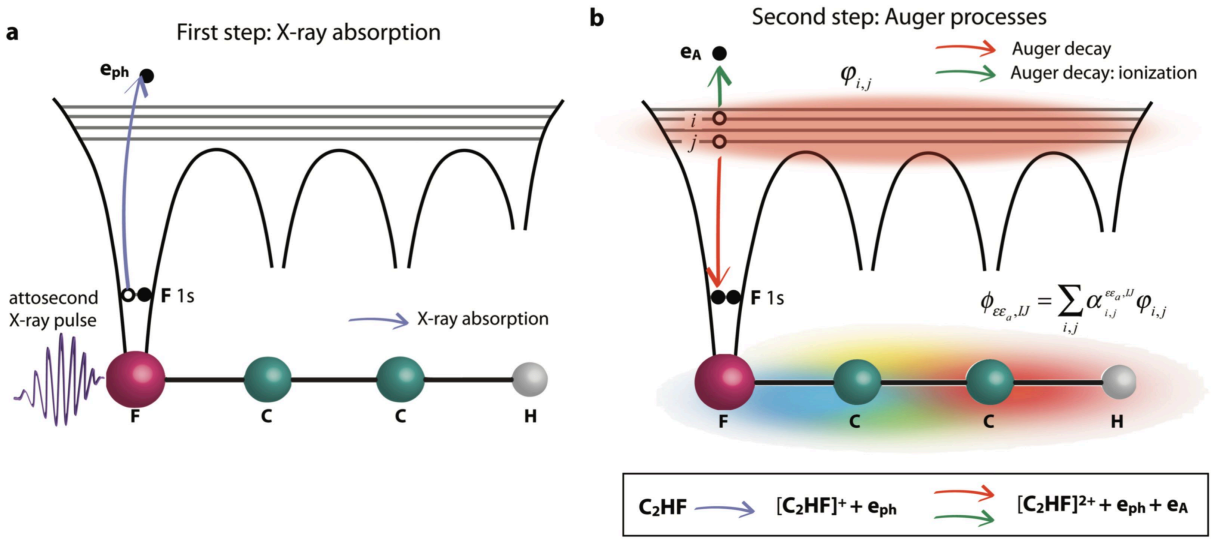

Figure 1: Auger-induced charge migration scheme in a fluoroacetylene molecule. a) An attosecond x-ray pulse ionizes the 1s electron at the F site. b) The Auger decay produces two holes in the valence shells that migrate along the molecule

[1] A. Picón *et al* 2016 *Nature Commun*. **7** 11652
[2] A. Picón, C. Bostedt, C. Hernández-García, and L. Plaja 2018 *Phys. Rev. A* **98** 043433