

SEMINAIRE ISMO

Victor Kimberg
PLEIADES, Synchrotron Soleil, Gif sur Yvette

Theoretical soft X-ray spectroscopy of nuclear dynamics in the presence of the vibronic coupling

Quite often excitation and de-excitation of the core-electrons induce nuclear dynamics resulting in unusual molecular phenomena. Already diatomic molecules exhibit interesting properties due to vibronic coupling of different core-excited or final electronic states, while polyatomic molecules show rich and nontrivial anisotropy properties. Owing to fast development of experimental techniques and technology in soft X-ray field during the last decades, it is now possible to explore vibrational structure of angle resolved spectra and thus probe nuclear motion of core-excited molecules with unprecedented details. In order to explain or predict the experimental results, adequate theoretical methods are required. Thereby, when few electronic states are vibronically coupled, it challenges theoretical approaches to go beyond the so-called adiabatic or Born-Oppenheimer (BO) approximation – one of the main concepts of molecular physics and chemistry. This allows revealing the dynamics of the molecular vibration in the presence of potential energy surfaces crossing and multichannel interference processes. In the present talk we will discuss a few examples of theoretical simulations of the non-BO behavior, which explain recent ultrahigh resolution experiments in gas-phase molecules related to angle-resolved photoion yield spectroscopy (ARPIS) [1], X-ray absorption spectroscopy (XAS) [2] and angle-resolved resonant Auger scattering (RAS) [3].

- [1] V. Kimberg, N. Kosugi, and F. Gel'mukhanov, "Theoretical studies of angle-resolved ion yield spectra of acetylene core-to-valence transitions." *J. Chem. Phys.* 130, 114302 (2009).
[2] Y. Velkov, V. Kimberg, N. Kosugi, P. Salek, and F. Gel'mukhanov, "Origin of fine structures on the dissociative $1s-s^*$ resonance in X-ray absorption spectra of O_2 ", *Chem. Phys. Lett.* 476, 147 (2009).
[3] C. Miron, V. Kimberg, P. Morin, C. Nicolas, N. Kosugi, S. Gavriluk, and F. Gel'mukhanov, "Vibrational scattering anisotropy generated by multichannel quantum interference", (submitted 2010).

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*Bât 351 - 2^{ème} étage -
Université Paris-Sud 91405 ORSAY Cedex*