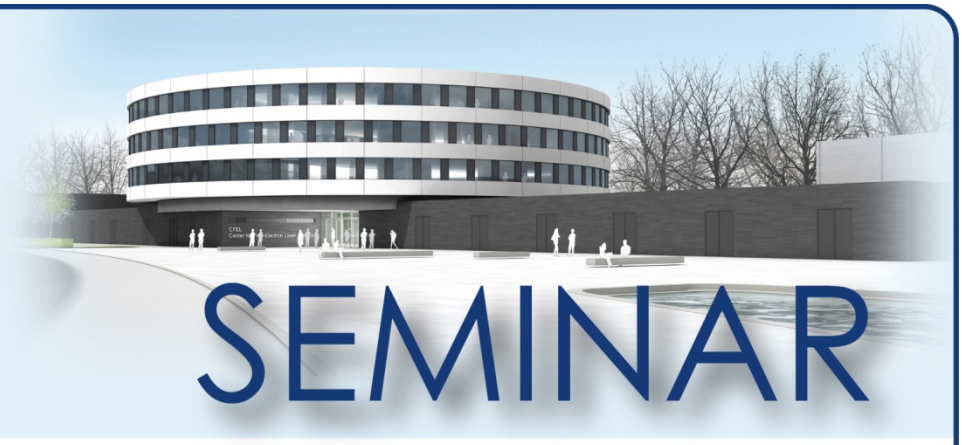
CFEL SCIENCE



SEMINAR

10th June 2011 - 11:15
Building 49 - Seminar Room 108

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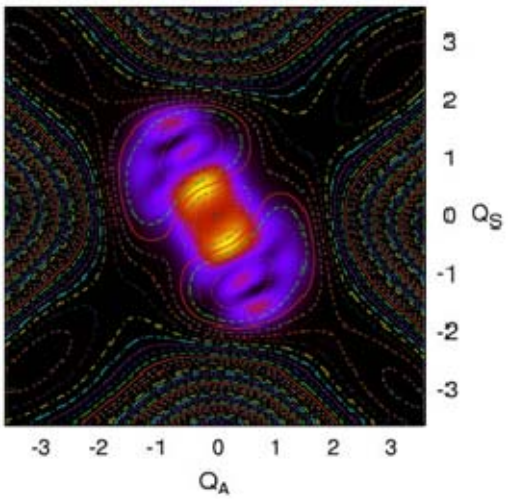
Core-hole induced nuclear dynamics studied by theoretical soft X-ray spectroscopies

Owing to the fast development of experimental techniques and technology in the area of soft x-rays over 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. The high complexity of the studied processes requires an adequate computational analysis for interpreting the experimental data. 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 theoretical approaches for studying the core-hole induced processes exhibiting non-BO behavior. Numerical simulations explain successfully the recent results on small 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].



Vibrational wave packet evolution in the 1s→π excited state of C_2H_2 leading to bent configuration. Core-hole lifetime is ~ 13 fs.*

[1] V. Kimberg, N. Kosugi, and F. Gel'mukhanov, J. Chem. Phys. 130, 114302 (2009).
[2] Y. Velkov, V. Kimberg, N. Kosugi, P. Salek, and F. Gel'mukhanov, Chem. Phys. Lett. 476, 147 (2009).
[3] C. Miron, V. Kimberg, P. Morin, C. Nicolas, N. Kosugi, S. Gavrilyuk, and F. Gel'mukhanov, Phys. Rev. Lett. 105, 093002 (2010).

Host: Nina Rohringer – MPG - ASG