Resonant Core Level Spectroscopies as Tools for Chemical Dynamics

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For larger and more complex molecules, one of the biggest challenges for experimental spectroscopy is in the interpretation of heavily convoluted spectra. X-ray spectroscopies and their element and site-selectivity can help address this challenge by providing observables that are uniquely related to particular atomic sites or functional groups in a system.

In this talk, I will discuss how, with combinations of complementary X-ray methods, it is possible to extract information on both electronic structure and dynamical processes on a series of molecular systems. I will look at how our recent developments for resonant X-ray techniques[1-3] are extending the chemically relevant information that can be extracted from these methods for polyatomics as well as providing insights into the few femtosecond processes following core-hole excitation.

1. D.M.P. Holland et al., "*Deconvolution of the X-ray Absorption Spectrum of trans-1,3-Butadiene with Resonant Auger Spectroscopy*", Phys. Chem. Chem. Phys. (26) 15130-15142 (2024)

2. E. Muchová, et al., "*Jahn–Teller effects in initial and final states: high-resolution X-ray absorption, photoelectron and Auger spectroscopy of allene*", Phys. Chem. Chem. Phys. (25) 6733-6745 (2023)

3. R.A. Ingle, et al., "*Carbon K-edge x-ray emission spectroscopy of gas phase ethylenic molecules*", J. Phys. B: At. Mol. Opt. Phys. (55) 044001 (2022)