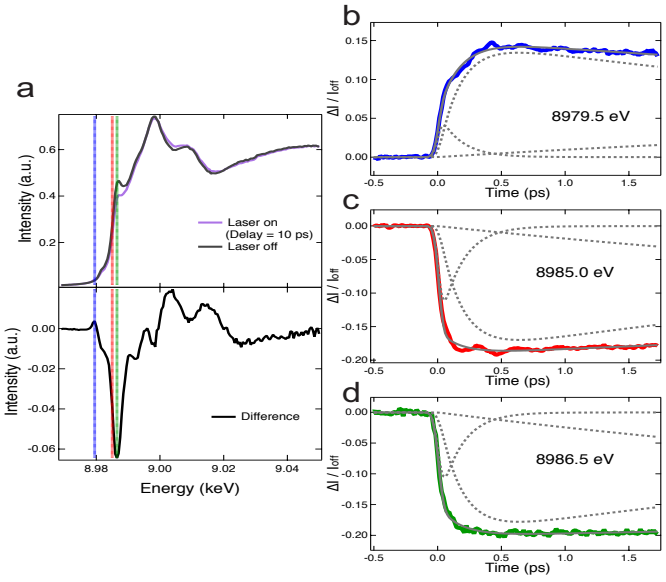
Probing Structure and Dynamics using Time-resolved X-ray Spectroscopy

Thomas J. Penfold[§]

[§] *Chemistry- School of Natural and Environmental Science, Newcastle University.*

Scientific breakthroughs are most commonly strongly associated with technology developments which enable the measurement of matter to an increased level of detail. A modern revolution is the quest to translate this ultrafast non-equilibrium dynamics into direct measurements of structural dynamics. This utilises the recent development of tools which deliver high-brilliance ultrashort pulses of X-rays, enabling methods that can achieve both high temporal (on the femtosecond time scale) and spatial (on the order on tenths of an angström) resolution.



Importantly, the complex nature and high information content of this class of techniques means that detailed theoretical studies are often essential to provide a firm link between the spectroscopic observables and the underlying molecular structure and dynamics. For X-FELs, understanding the femtosecond dynamics of molecules in electronically excited states requires simulations that go beyond the single nuclear configuration regime and the Born-Oppenheimer approximation.

Herein I will present some recent work on simulating and understanding ultrafast X-ray spectra using excited state simulations based upon quantum nuclear dynamics. This will include prediction and experimental realisation of ultrafast time-resolved experimental signals of a Cu transition metal complex (Figure 1) and metal oxide nanoparticles. Future perspectives and opportunities will also be discussed.

1. T. J. Penfold, E. Gindensperger, C. Daniel and C. M. Marian, Chem. Rev., **118**:6975 (2018).
2. G. Capano, C.J. Milne M. Chergui, U. Rothlisberger, I.Tavernelli and T.J. Penfold J. Phys. B **48**:214001 (2015).