Warwick Chemistry Departmental Seminar

Dr Tom Penfold

University of Newcastle

Thursday 21 February

4.00 pm, Physics Lecture Theatre, Science Concourse

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

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 and metal oxide nanoparticles. Future perspectives and opportunities will also be discussed.

Biography

Tom started the position of lecturer in theoretical chemistry at Newcastle in September 2015. He completed his PhD in 2010 at the University of Birmingham, supervised by Graham Worth. After this he spent 3 years at the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland in the group of Majed Chergui. He worked in close collaboration with the experiments performed within the group, analysing and understanding their data, particularly static and time-resolved X-ray absorption spectroscopy. He then moved to the Paul Scherrer Institute, Switzerland, working as a research scientist on the Swiss Free Electron Laser Project developing computational approaches for simulating and interpreting femtosecond time-resolved X-ray absorption and emission experiments. Research in his group focuses on understanding excited state processes and dynamics at a molecular level with the ultimate goal to use this fundamental knowledge to design better and more efficient solar cells, photocatalysts and/or light emitting diodes. **Area of Expertise:** Excited State Dynamics and Time-resolved Spectroscopy.