



YCCSA Seminar Series Autumn 2018

An interdisciplinary seminar series hosted by the York Cross-disciplinary Centre for Systems Analysis aimed at researchers from all disciplines

Ultrafast 2D-IR Spectroscopy – Challenges for Real World Biomolecular Applications

Professor Neil Hunt

Physical Chemistry, York

Friday, 19 October 2018

Ron Cooke Hub, RCH/204 at 13:30

Abstract:

Two-dimensional infrared spectroscopy (2D-IR) is an ultrafast, non-linear optical spectroscopy method that has grown steadily in stature and usage since the first demonstration of the technique around two decades ago. In particular, 2D-IR spectroscopy has found many applications in investigating the structure, dynamics and intermolecular interactions of biological molecules in the solution phase. Advances in laser technology now mean that it is possible to acquire 2D-IR spectra in a few seconds, meaning that high throughput applications of 2D-IR in the drug design process are realisable. However, current spectral analysis methods cannot keep pace with spectral acquisition meaning that novel approaches to data analysis are required if we are to realise the full potential of the 2D-IR method. The aim of this presentation is to give an introduction to the method of 2D-IR using examples to illustrate the way in which 2D-IR spectroscopy has expanded our view of dynamic biomolecules in solution. Preliminary tests of high throughput 2D-IR screening experiments and initial data analysis strategies will be described, hopefully creating a basis for further discussion.

The seminar includes a refreshment break to fuel interdisciplinary discussion

Ron Cooke Hub is on Heslington East Campus – accessible by free bus services

Nos. 66 and UB1 running at frequent intervals from Heslington West.

The YCCSA Seminar room is on the second floor