Contribution ID: **21** Type: **Contributed Talk**

A combined experimental and theoretical study of the excited state dynamics of a prototypical Cu(I)-phenanthroline complex

Tuesday 16 September 2014 12:35 (25 minutes)

Cu-phenantholine complexes are promising candidates for photoelectronic applications. However, despite being extensively studied since the early '80s, a complete understanding of their photophysical and photochemical properties is still lacking. In particular, both the mechanism by which luminescence quenching occurs in donor solvents and the nonadiabatic relaxation processes in the low lying singlet and triplet MLCT excited states are hotly debated. I will present a combined time-resolved X-ray absorption spectroscopy and theoretical study of a prototypical Cu(I)-phenanthroline complex [Cu(dmp)2]+ (dmp = 2,9-dimethyl-1,10-phenanthroline), aimed at elucidating the excited state mechanisms occurring within the femto- to nanosecond time domains.

In the pico and nanosecond domain, time-resolved XAS does not confirm the previous assignment of excited state lifetime shortening in donor solvents (acetonitrile) to a metal centred exciplex. Instead, the lifetime quenching of the title complex and related complexes may be rationalised by the solvent induced decrease of the triplet MLCT energy.
In the femtosecond time domain, we employ the Multi Configurational Time Dependent Hartree method to explore the nonadiabatic relaxation of [Cu(dmp)2]+ following excitation into the S3 state. The results, in conjunction with previous experiments allow us to rationalise the ultrafast dynamics of this complex and shed insight into the relaxation of the system to the long live triplet state.

Primary author: PENFOLD, Thomas

Presenter: PENFOLD, Thomas

Session Classification: Chemistry

Track Classification: Chemistry