**Ultrafast Structural Dynamics of Light-Driven Charge Transfer in Photoactive Metal Complexes with Controllable Reactivity**

A fully-funded 4-year PhD position is available from 1 October 2020,
in the group of Professor Julia Weinstein at the University of Sheffield, UK.

**BACKGROUND:** Control of light-driven charge- and energy transfer in photoactive molecules and materials – directing reactivity at will – is a fascinating challenge in chemistry and photosciences.

We have recently shown that, contrary to the accepted view, it ***is*** possible to control photoinduced electron transfer in solution, by targeted infrared excitation of selected molecular vibrations on the ultrafast timescale. We demonstrated this effect of "IR-control" for electronic excited states of light-harvesting transition metal complexes of the type [Donor]-bridge-[acceptor]. [see for example *Science* 2014, 1492; *Nature Chem* 2017, 1099]

The PhD project aims to take the next step: to develop fundamental understanding of the mechanism of this exciting effect. The key questions include the role of vibronic coupling, coherence, and structural changes accompanying electronic excitation in such systems in solution, on the ultrafast, sub-20-ps, time scale. To answer these questions, we will combine ultrafast optical spectroscopy methods with emerging methods of ultrafast structural dynamics (such as femtosecond X-ray absorption and emission from molecules *in solution*) made possible by X-ray Free Electron Lasers, XFEL.

The combination of ultrafast optical spectroscopy and XFEL can bring fundamentally new insights into electronically excited states of transition-metal complexes, which underpin broad range of their applications, ranging from solar energy conversion and photocatalysis, to electron transfer in biochemistry.

**PROJECT:** The scientific aim of the PhD will be understanding, with femtosecond time-resolution and atomistic spatial resolution, of ultrafast structural dynamics accompanying light-induced charge transfer in metal complexes in solution, and understand the mechanism of the "IR-control" effect.

The PhD will initially focus on the complexes of Pt(II) and Cu(I) which show potential for controllable photochemistry on sub-picosecond timescale. These compounds will be first studied in detail by femtosecond optical spectroscopies in The Lord Porter Laser Laboratory at the University of Sheffield, https://www.sheffield.ac.uk/laser-spectroscopy. The lab comprises ultrafast (~40 fs) transient absorption spectroscopy, ultrafast broadband Fluorescence Upconversion spectroscopy, and ultrafast transient infrared (TRIR) spectroscopy with the capability for multipulse experiments (2DIR and UV/IR/IR pulse-sequences). The PhD student will routinely use these methods. They will also have an opportunity to contribute to the development of new set-ups and methods in Sheffield. The work on ultrafast structural dynamics will be done via access to, and collaboration with, the European XFEL (FXE), and SwissFEL.

The project could help answering the questions on the role and mechanism of vibronic coupling and coherent energy transfer in metal complexes in solution, and in turn help developing "IR-control" as a way to direct photo-reactivity.

The student will join an international, interdisciplinary, and dynamic group of PhD students and postdocs located in the Department of Chemistry at the University of Sheffield, and become part of the LaserLab community. We collaborate on computational chemistry with the group of Professor A. Meijer in Sheffield, and with the National (STFC, Diamond) and international research facilities.

**Sheffield** is the UK's greenest city, situated at the edge of the Peak District National park with plenty of the opportunities for cycling, climbing, and hiking. The University of Sheffield, www.sheffield.ac.uk, is a world top-100 university and world top 50 most international. Sheffield is located in the center of the UK, with direct train connections to London (2 h), Manchester (1h) and York (1h).

**REQUIREMENTS:**

The candidate should have a 1st or an upper 2nd class degree (or an equivalent) in Physics, Chemical Physics, or Physical Chemistry. Expertise in working with ultrafast amplified lasers is strongly desirable. Enthusiasm, willingness to travel to conduct experiments, and ability to work independently in an interdisciplinary setting are essential.

The PhD position is jointly funded by UK XFEL Physical Sciences Hub and the University of Sheffield. The position is funded for 4 years, all tuition fees are covered. The position is open to EU/UK residents.

Start date: 01 October 2020.
Application deadline: The position will be advertised until filled.

**Informal inquiries:**
Professor Julia Weinstein, jullia.weinstein@Sheffield.ac.uk.
https://www.sheffield.ac.uk/chemistry/people/academic/julia-weinstein

**Laser laboratory:** https://www.sheffield.ac.uk/laser-spectroscopy

**Formal applications:** https://www.sheffield.ac.uk/postgraduate/how-apply-0

**References:**

1. Delor M, Archer SA, Keane T, Meijer AJHM, Sazanovich IV, Greetham GM, Towrie M & Weinstein JA (2017) **Directing the path of light-induced electron transfer at a molecular fork using vibrational excitation**. *Nature Chemistry*, 9(11), 1099-1104.

2. Scattergood PA, Delor M, Sazanovich IV, Towrie M & Weinstein JA (2015) **Ultrafast charge transfer dynamics in supramolecular Pt(II) donor–bridge–acceptor assemblies: the effect of vibronic coupling**. *Faraday Discussions*, 185, 69-86.

3. Delor M, Keane T, Scattergood PA, Sazanovich IV, Greetham GM, Towrie M, Meijer AJHM & Weinstein JA (2015) **On the mechanism of vibrational control of light-induced charge transfer in donor–bridge–acceptor assemblies**. *Nature Chemistry*, 7(9), 689-695.

4. Delor M, Sazanovich IV, Towrie M & Weinstein JA (2015) **Probing and Exploiting the Interplay between Nuclear and Electronic Motion in Charge Transfer Processes**. *Accounts of Chemical Research*, 48(4), 1131-1139.

5. Delor M, Scattergood PA, Sazanovich IV, Parker AW, Greetham GM, Meijer AJHM, Towrie M & Weinstein JA (2014) **Toward control of electron transfer in donor-acceptor molecules by bond-specific infrared excitation**. *Science*, 346(6216), 1492-1495.