Master in Photonics – "PHOTONICS BCN"
ERASMUS+ "EUROPHOTONICS"

MASTER THESIS PROPOSAL

Dates: April - September 2021

Laboratory : Attoscience and Ultrafast Optics
Institution: ICFO – The Institute of Photonics Sciences
City, Country : Barcelona, Spain

Title of the master thesis: Molecular structural imaging with single-electron diffraction

Name of the master thesis supervisor: Prof. Dr. Jens Biegert
Email address: jens.biegert@icfo.eu
Phone number: +34935534059
Mail address: ICFO - The Institute of Photonics Sciences, The Barcelona Institute of Science and Technology, Av. Carl Friedrich Gauss 3, 08860 Castelldefels (Barcelona), Spain.

Keywords: attosecond science, electron diffraction, structural identification, molecular dynamics, diffraction imaging.

Summary of the subject (maximum 1 page):

Conventional electron and X-ray diffraction have identified the geometric structures of many biologically-important molecules. For example, the structure of DNA, which eluded scientists for many decades, was measured using X-ray diffraction in 1952 by Franklin and Gosling which steered the model of Watson and Crick to identifying its double-helix structure in 1953. In fact, many biological processes are driven by chemical reactions, but their reaction mechanisms are still unknown with many different reaction pathways proposed. One such chemical reaction is *trans-cis* photoisomerization of photo-switchable molecules possessing geometric isomerism which, for example, help regulate vision and metabolism.

To resolve the structure of molecules in chemical reactions, an imaging technique is required that can capture a clean snapshot of molecular structure with atomic spatial (*i.e.* Ångstrom; 1 Å = 10^{-10} m) and temporal (*i.e.* femtosecond; 1 fs = 10^{-15} s) resolution. This is achieved using laser-induced electron diffraction (LIED) which can directly retrieve the structure of gas-phase molecules with sub-atomic picometre (1 pm = 10^{-12} m) and attosecond (1 as = 10^{-18} s) resolution.

You will be dealing with the theory and method of LIED to directly identify and distinguish the static structures of *trans*- and *cis*- isomers. This will provide the starting and end points of the *trans-cis* photoisomerization reaction, the data from which will then be utilized to identify the transient structures in future time-resolved pump-probe measurements of isomerization. We will then explore opportunities of improving structural retrieval with LIED, for example, by increasing the number of scattered electrons generated through the addition of a second, weak laser pulse in two-pulse LIED measurements.

LIED imaging works by using an intense, femtosecond laser pulse to emit an electron from a molecule through quantum tunnel ionization. The emitted electron is then accelerated and returned by the oscillating electric field of the laser pulse to subsequently elastically scatter and diffract against the molecular ion. The scattered electrons are then detected in coincidence with the ion of interest using a high-resolution particle detector, called a reaction microscope. Structural information embedded in the detected three-dimensional momentum distribution of the scattered electrons is then directly retrieved to identify the molecular structure. LIED imaging has successfully directly imaged deprotonation reactions in molecules, the strong nuclear-electronic coupling *via* the Renner-Teller effect, and the structural identification of many small gas-phase molecules. An exciting opportunity now exists to extend LIED imaging to more complex, larger polyatomic molecules which possess a rich variety of chemistry.

Additional information:

***Required skills:** Physics or Physical Chemistry undergraduate, problem-solving, critical-thinking, quick learner, ability to work independently and in a team, basic computer programming.

***Miscellaneous:**