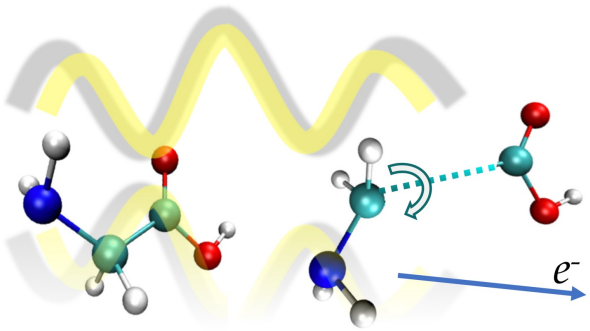
School on "Ultrafast phenomena in Chemistry: Laser-matter interactions at the femto- and atto-second time scales"



Dates: **May 22nd-26th, 2023**

Contact: alicia.palacios@uam.es

Description: This subject will introduce the most fundamental concepts for **ultrafast chemistry**. This course provides a solid background on the theoretical aspects to describe the **interaction of laser pulses with matter**. It is designed with a set of comprehensive **tutorials** to learn how to describe the ultrafast electron and nuclear dynamics triggered in distinct scenarios, from traditional weak-field approaches to strong field light-induced phenomena. The contents are designed to first introduce pulse characterization techniques and signal analysis in experiments where coherent light pulses interact with molecules. It is then followed by four practical sessions with open source codes for the description of light in time and frequency domains, and its interaction with molecular targets, using simplified models and different laser parameters. An extensive tutorial and practical sessions will be provided on DFT and TDDFT approaches (**OCTOPUS software**) to describe the **light-induced phenomena in large molecules and biomolecules**.

The contents and practical sessions are designed for students at Master level or first year of PhD in the areas of Chemistry and Physics, including theoretical quantum chemists, experimental chemists and physicists working with light sources, and most related areas in the field of atomic and molecular physics and chemistry and optics. It has been planned with **hands-on tutorials, performed in the computer lab, learning the methods and basic concepts to describe the first steps in photo-induced phenomena in molecules**.

This school will provide a complete formation on theoretical methods to describe light-induced phenomena in molecules, thus setting up a solid background to further connect related topics and concepts, as those taught in closely related and more specific subjects such as "Excited states Chemistry: Quantum and Mixed Quantum Classical Dynamics in Photochemistry" and "Kinetics and Dynamics of Chemical Reactions".

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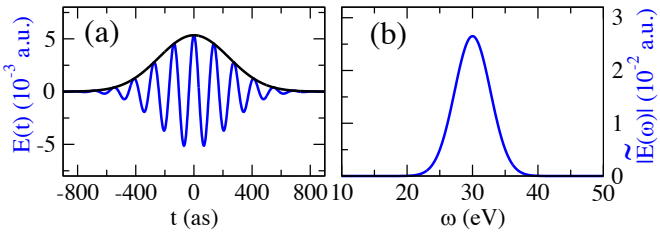
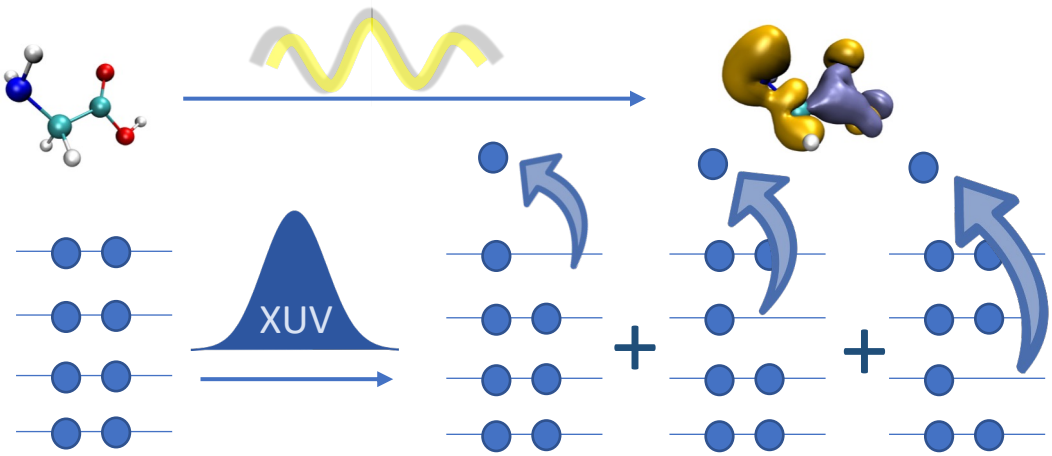
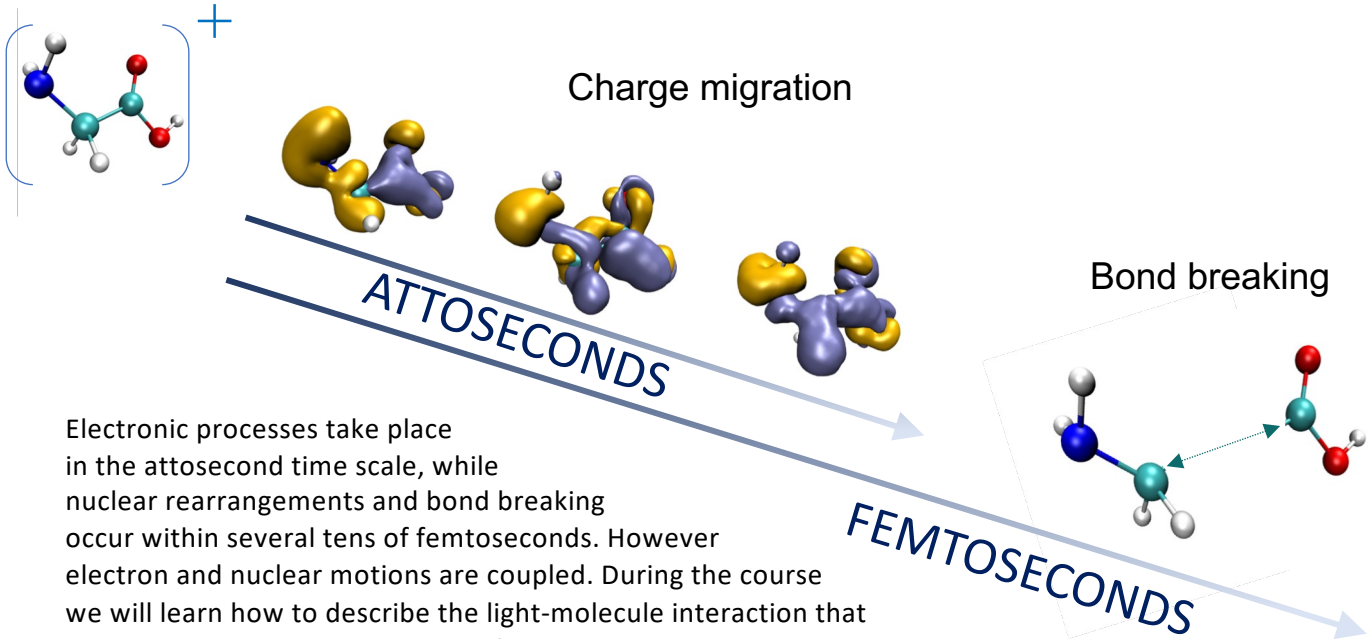
The field of Femtochemistry has greatly evolved over the last 30 years. In the first part of this course, we will learn how to theoretically describe the light sources that are used in current experiments to obtain time-resolved images of photochemical reactions in real time.



Ultrashort laser pulse in time and frequency domains.



Electrons are ejected from different molecular orbitals creating an electronic wave packet in a few tens of attoseconds. In the course, we will learn the fundamental concepts and numerical implementations (e.g., time propagation schemes) to describe this ultrafast dynamics.



Electronic processes take place in the attosecond time scale, while nuclear rearrangements and bond breaking occur within several tens of femtoseconds. However electron and nuclear motions are coupled. During the course we will learn how to describe the light-molecule interaction that triggers this dynamics. The state-of-the-art methodologies will be introduced.

cecam
Centre Européen de Calcul Atomique et Moléculaire

Lecturers

Jens Biegert

Group Leader at ICFO (Instituto de Ciencias Fotónicas, Barcelona).

More info:
J Biegert's website

Expertise: Experimental group "Attoscience and Ultrafast Optics" working on Attosecond X-ray Science, Extreme Photonics, Quantum Dynamics & Ultrafast Laser Science. Ongoing research funded by the prestigious ERC Advanced Grant "TRANSFORMER" (~2,5 million €), exploring real-time electronic and nuclear dynamics of molecular transformations and phase transitions.

Johannes Feist

Group Leader at Univ. Autónoma de Madrid.

More info:
J Feist's website

Expertise: Research on polaritonic chemistry, i.e., the manipulation of chemical structure that can be achieved through strong coupling between confined light modes and organic molecules. This ongoing research funded by the prestigious ERC Starting Grant MMUSCLES (~1,5 million €). Long expertise on Attosecond Science and High performance computing.

Wojciech Gawelda

Distinguished Professor *Beatriz Galindo* at Univ Autónoma de Madrid & Associate Researcher at IMDEA Nanociencia.

More info:
W Gawelda's website

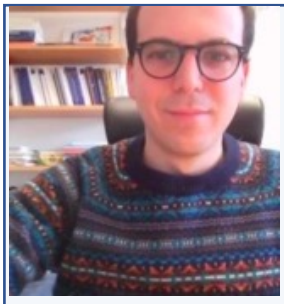
Expertise: Experiments using ultrafast X-ray techniques in combination with ultrafast optical spectroscopies to study photoinduced structural dynamics in chemical systems, mainly solvated transition metal complexes. Long career developed at the Femtosecond X-ray Experiments Group at the European XFEL In Hamburg (Germany) as Senior Staff Scientist (2010-2020).

Carlos Hernández

Associate Professor at Universidad de Salamanca.

More info:
Hernández's website

Expertise: Expert on developing the theoretical formalism and methods to investigate the light structure properties (e.g., angular momentum properties) in high-order harmonic generation (HHG) techniques, as well as its interaction with matter. This ongoing research is funded by the prestigious ERC Starting Grant ATTOSTRUCTURA (~1,4 million €).



Felipe Zapata

Dr "Margarita Salas" at Lund Univ. and Univ. Autónoma de Madrid.

More info:
Portal at Lund

Expertise: Young post-doctoral researcher holding a national competitive "Margarita Salas" Fellowship for Lund (Sweden) and Madrid (Spain). Research on photoinization processes in atomic systems accounting relativistic effects. Light-matter interactions using ultrashort pulses. Code developer.

Alberto Castro

Group Leader at BIFI Universidad de Zaragoza.

More info:
A Castro's website

Expertise: Research at the Institute for Biocomputation and Physics of Complex Systems. Electron dynamics using time-dependent density functional theory TDDFT using quantum optical control theory and exploring non-adiabatic molecular dynamics. One of the **founding authors of** OCTOPUS software platform, and still an active developer and performing applications.

Alicia Palacios
(Coordinator)

Associate Professor at Univ. Autónoma de Madrid

More info:
A Palacios's website

Expertise: Developer of ab initio time-dependent treatments to describe atoms and molecules subject to ultrashort intense laser pulses. Long trajectory employing high performance computing to investigate non-linear phenomena in Atto- and Femtochemsitry. Her trajectory was awarded with the Mildred Dresselhaus Junior Award 12018 from Hamburg University.