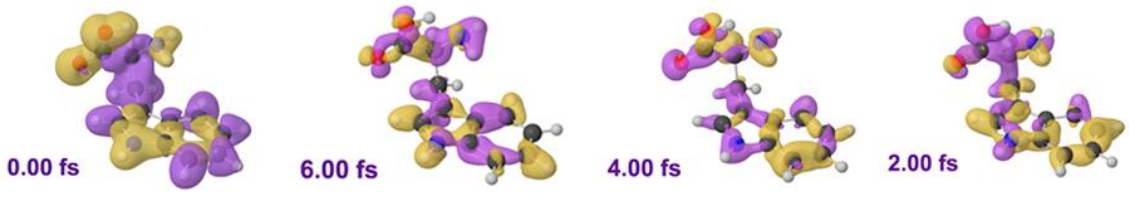
Theoretical modelling of attosecond dynamics induced by X-ray free-electron lasers

About the project

X-ray free-electron lasers (XFELs) are nowadays able to deliver few-femtosecond and sub-femtosecond light pulses in the XUV and X-Ray frequency regions, which allows one to investigate, for the first time, the ultrafast electronic dynamics triggered in atoms, molecules and materials at its natural time scale, the attosecond. The goal is to attain control at the ultrashort time scale by manipulating in real time the motion of electrons and atomic nuclei. In brief, the electron hole created after ionization by such pulses freely evolves for a few femtoseconds until, later on, it is coupled to the slower nuclear motion leading to geometrical changes in the molecular structure and/or fragmentation. This can yield localization of the charge in specific fragments. As a result, these experiments seek to attain control on chemical reactivity by tailoring the laser pulses (phase and amplitude) at the attosecond time scale.

The IMDEA-Nano group is world expert in developing theoretical methods to describe ionization processes as those induced by XFELs (see, e.g., https://campusys.qui.uam.es/). These methods rely on the ab initio solution of the time dependent Schrödinger equation, which requires the use of advanced supercomputers, such as those available at the European Supercomputer network, among them the Mare Nostrum Supercomputer in Spain. Most of the methods that will be used are already available in the group.

The project will provide theoretical support to ongoing and future experiments performed at the European XFEL (https://www.xfel.eu/), with which IMDEA Nano is associated through a recent agreement. Therefore, although the research will be 100% theoretical, it will be performed very close to actual experimental measurements and/or will be used to predict new physical phenomena that could be observed in XFEL facilities and eventually to design new experiments. Collaboration with the theory groups of IMDEA Nano and Universidad Autónoma de Madrid working in these topics will be straightforward. Secondments at the European XFEL in Hamburg will be offered in order to assist experimental measurements inspired by the theoretical modelling. Theoretical training will be provided through some of the schools organized by the AttoChem European network (https://attochem.qui.uam.es/), coordinated by the IMDEA group, such as the Erice School in Attosecond science and the Zaragoza School in Theoretical Attosecond methods.



See also the AttoChem videos at https://www.youtube.com/watch?v=5n5l7mJ-BCY&list=PLZdQHnbBuXc-CxblhWm6pXUQNEwWhCiTK&index=1.

For further information about the project please contact the project lead Prof. Fernando Martín (fernando.martin@imdea.org) and visit https://idealcofund-project.eu/phd/phd-projects/theoretical-modelling-of-attosecond-dynamics-induced-by-x-ray-free-electron-lasers/.

❖ Applicant´s requirements

Bachelor or Master in Physics or Theoretical Chemistry, with basic knowledge of operating systems, preferentially linux, and programming in Fortran, C, C++ or Python. Inclination for theoretical research and mathematical developments.

To be positively valued:

- Proactivity
- Enthusiasm and creative thinking
- Ability to work autonomously under group-oriented strategy

❖ How to apply

Application deadline: 10 April 2023 (17:00 CET)

This project is part of the IDEAL PhD Fellowship Programme led by Fundación IMDEA Nanociencia and co-funded by the **Marie Skłodowska-Curie Actions (MSCA) COFUND programmes.** IDEAL PhD will offer 12 fellowships in two open calls to outstanding doctoral candidates to undertake a PhD research project in any of the programmes at the Institute. More information at IDEAL PhD Fellowship programme**.**

Applicants must submit their applications through the IDEAL PhD Fellowship Programme website. Before submitting your application, please download and check the Guide for Applicants and templates.

❖ About IMDEA Nanociencia

The IMDEA Nanoscience Institute, created in 2006 at the initiative of the Community of Madrid, is an interdisciplinary research centre dedicated to the exploration of basic Nanoscience and the development of nanotechnology applications in connection with innovative industries. IMDEA Nanociencia has been a "Severo Ochoa" Centre of Excellence since 2017, this is the highest national recognition for scientific excellence granted by the Ministry of Economy, Industry and Competitiveness. The Institute is located and forms part of the UAM-CSIC Cantoblanco Campus of International Excellence, a highly competitive research environment worldwide.