

PhD position on ultrafast molecular dynamics induced by attosecond pulses

Research Center: Condensed Matter Physics Center (IFIMAC) - <http://www.ifimac.uam.es/>

Center Description: The IFIMAC Center is a new María de Maeztu Excellence Research Unit located in the campus of the Universidad Autónoma de Madrid pursuing cutting-edge research and scientific excellence.

Area of knowledge and discipline: PHYSICAL SCIENCES, MATHEMATICS and ENGINEERING panel. PHYSICS

Project Title: Ultrafast molecular dynamics induced by attosecond pulses.

Group leader: Prof. Fernando Martín García. CampuS Theoretical Group (<https://campusys.qui.uam.es/>)

Research project / Research Group description:

Since the generation of the first attosecond pulse in 2001, the progresses in attosecond laser technology in conjunction with advanced photo-fragment detection techniques as velocity map imaging (VMI) and cold target recoil-ion momentum spectroscopy (COLTRIMS) has enabled unprecedented experimental capabilities to retrieve time-resolved images of electron dynamics in atoms and molecules. Molecular targets are particularly interesting, involving processes occurring in the attosecond time scale (electron dynamics) to the femtosecond time scales (from slow electronic processes to molecular vibration and dissociation). A deep understanding of the electron dynamics that is initiated by attosecond pulses can be only achieved by means of quantum mechanical description of the laser-atom and laser-molecule interactions.

The CampuS research group has demonstrated its international leadership providing accurate and predictive theoretical methods to explore ultrafast processes in small molecules. The capabilities of our almost exact theoretical tools are demonstrated through our most recent works on atoms and small molecules, a significant part of them in close collaboration with experimental groups, and published in the most prestigious international journals such that Nature 516, 374 (2014), PNAS 111, 3973 (2014), PNAS 111, 912 (2014), Science 346, 336 (2014), Phys. Rev. X 5, 041053 (2015), Science 354, 734 (2016); Nature Comm. 7, 10566 (2016), Physical Review Letters 117, 093003 (2016) or Chem. Rev. 117, 10760 (2017).

The main objective of this project is to retrieve time-resolved images of the coupled electron and nuclear dynamics in light molecules, specifically addressing unsolved problems (i.e. multiphoton double ionization of small diatomic molecules or dissociation into neutrals upon autoionizing). To achieve this goal, it will be required the development and extension of state-of-the-art time-dependent ab initio approaches describing the molecular targets in full dimensionality.

Job position description:

The fellow will develop a research project on “Ultrafast molecular dynamics induced by attosecond pulses”, oriented to obtain a PhD diploma. Ab initio theoretical methods will be implemented to explore the coupled electron and nuclear dynamics induced by attosecond laser pulses in small molecules. Unexplored multiphoton ionization processes induced by ultrashort laser sources such that high-harmonic generation and free-electron laser facilities will be investigated in collaboration with international experimental groups.

Full dimensional ab initio methodologies will be extended and implemented using parallel computation, in particular Message Passing Interface (MPI), using the supercomputers available through the European HP Computing Network. Research stays with collaborating groups and attendance to international conferences are foreseen.

Candidates should fulfill the call requirements and have a solid background in quantum mechanics and its mathematical foundations and a related master degree; a mature interest in the implementation of new computational tools, including good knowledge of programming languages (Fortran 90, C, C++, Python, etc.); enthusiasm for learning and commitment to teamwork.

We will positively value any additional skills in the areas of mathematics, physics and computation that are relevant to the offered position. For example, participation to software projects; competences in photoelectron spectroscopies, attosecond physics; etc. Other IT competences as knowledge of scripting languages, graphical programs and numerical libraries will be also taken into account.

Related link to the position:

XChem European Research Council project: <https://www.xchem.uam.es/xchem/>