Theoretical Attosecond Electron Dynamics: from biomolecules to solids

IMDEA - Nanociencia Institute
www.nanociencia.imdea.org

CENTRE DESCRIPTION

IMDEA Nanociencia is a young interdisciplinary research centre dedicated to the exploration of basic nanoscience and the development of applications of nanotechnology in connection with innovative industries.

Our purpose-built building was inaugurated in 2014 and features state-of-the-art facilities for 21st century science, where the frontiers between fields disappear and Physics, Chemistry, Biology, Engineering, and Medicine merge. It features more than 30 operative laboratories with over € 16 M worth of equipment - including the Centre for Micro and Nanofabrication. We are located at the UAM Campus, with access to all the facilities of one of Spain's largest and most prestigious Universities. The UAM Campus is just a few minutes away from Madrid's lively city centre, connected by "cercanías" trains and several bus lines.

We are over 150 scientists, with different professional and personal backgrounds. Approximately 40% of our PhD and postdocs come from outside Spain, representing every corner of the world, from Germany to China, from the USA to Singapore –a true international environment in which to develop your scientific career. Women make up 36% of our scientific and 62% of our management staff. No matter who you are or where you come from, you will feel welcome from the very first minute.

We take science seriously and value quality over quantity. Our scientists enjoy tackling complex multidisciplinary problems, often within in-house collaborations, so all of our students receive truly interdisciplinary training. We also enjoy publishing in the very best journals, with >200 publications a year, and an institutional h index of 79. Check out our webpage http://nanociencia.imdea.org/, facebook @IMDEANanociencia or twitter @IMDEA_Nano for more information.

So if you are a talented, hard-working individual with a real interest in Science, IMDEA Nanociencia is the right place for you! Come work with us!

ADDRESS

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AREA OF KNOWLEDGE

Physical Sciences, Mathematics and Engineering

GROUP OF DISCIPLINES

Physics

GROUP LEADER

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Research Group Website: http://nanociencia.imdea.org/fernando-martin-s-group/group-home

Research project/ Research Group description

Dynamical processes in biomolecules and condensed matter occur on an ultrafast temporal scale, ranging all the way from picoseconds to femtoseconds, when considering structural changes, and down to attoseconds, when dealing with electrons. Electron dynamics and its interplay with the nuclear motion play a very important role in bond-formation and bond-breakage, thus determining chemical reactivity. Therefore, by acting on the system on this ultrafast time scale, e.g., by using attosecond light pulses on molecules, one could in principle manipulate the molecule's charge distribution and consequently induce bond breaking at different molecular sites. Although much progress has been done in the last few years to image charge delocalization in molecules in the gas phase, interpretation of actual measurements and design of control strategies is seriously limited due to the large number of electronic and nuclear degrees of freedom involved in those processes. The situation is even worse in solids.

The implementation by the research group of accurate quantum mechanical time-dependent theoretical methods in supercomputers has made it possible to guide experimental research in this field since its birth at the beginning of this decade. As an example, see recent results published by the group in *Chem. Rev.* **117** (2017) 10760; *Nature* **516** (2014) 374, *Science* **354** (2016) 734; *Science* **346** (2014) 336, *Nature Comm.* **7** (2016) 10566, *Nature Comm.* **8** (2017) 2266, *Nature Physics* **14** (2018) 733, *Physical Review Letters* **117** (2016) 093003, *Physical Review Letters* **121** (2018) 103002, *Scientific Reports* **6** (2016) 32653, *Science Advances* **4** (2018) eaat3962 or *Phys. Rev. X* **5** (2015) 041053.

The objective of the project is to study attosecond and sub-femtosecond electron and nuclear dynamics in biomolecules and solids, by developing new time-dependent computational tools and novel concepts that allow one to rationalize the use of ultra-short light sources for imaging and controlling such dynamics.

Job position description

The fellow will develop a research project on "Theoretical Attosecond Electron Dynamics in biomolecules and solids", oriented to obtain a PhD diploma and in close collaboration with the CampuS research group (https://campusys.qui.uam.es/). The main goal is to theoretically investigate ultrafast processes such that ultrafast charge migration induced by attosecond laser pulses and strong electromagnetic fields.

New theoretical tools in combination with quantum chemistry packages (from DFT to post-Hartree Fock methods) will be designed to describe the unexplored ultrafast phenomena arising in such large targets. The successful applicant will collaborate with internationally recognized theoretical and experimental research groups in the area of Atomic, Molecular and Optical Physics. Scientific stays in the collaborating groups and attendance to worldwide conferences are foreseen.

Apart from the specific call requirements, candidates should 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 chemistry that are relevant to the offered position. For example, acquaintance with atomic and molecular structure computational packages; 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.

The ideal candidate should have a master in Condense Matter Physics, in Theoretical Chemistry, or similar area. Knowledge of PBC simulation packages and programming skills are desirable but not mandatory. Good knowledge of English and teamwork skills are required.

OTHER RELEVANT WEBSITES

https://campusys.qui.uam.es/