PhD position on Theoretical Attosecond Electron Dynamics: from biomolecules to solids

Research Center: FUNDACION IMDEA NANOCIENCIA - http://www.nanociencia.imdea.org/

Center 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. IMDEA Nanociencia has been recently selected as Severo Ochoa Centre of Excellence.

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

Project Title: Theoretical Attosecond Electron Dynamics: from biomolecules to solids
Group leader: Prof. Fernando Martín García. 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, Physical Review Letters 117 (2016) 093003, Scientific Reports 6 (2016) 32653 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 on biomolecules and first applications on solids.
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 application will collaborate with internationally recognized theoretical and experimental research groups in the area of Atomic, Molecular and Optical Physics. Short-term scientific stays in the international collaborating groups and attendance to world-wide 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 valued 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.

Related links to the position:
XChem European Research Council project: https://www.xchem.uam.es/xchem/
CampuS theoretical research group: https://campusys.qui.uam.es/