PhD position on Theoretical Attosecond Electron Dynamics

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: PHYSICAL SCIENCES, MATHEMATICS and ENGINEERING panel

Disciplines: PHYSICS

Project Title: Imaging and control of electron dynamics with attosecond laser pulses

Group leader: Prof. Fernando Martín García. CampuS Theoretical Group.
https://campusys.qui.uam.es/ (Computations in Atomic and Molecular Physics of Unbound Systems)

Research project / Research Group description:

Dynamical processes in molecules 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. Both electronic and nuclear dynamics 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 CampuS 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 *Nature* **516** (2014) 374, *Science* **346** (2014) 336, Nature Photonics **9** (2015) 76, *Nature Comm.* **7** (2016) 10566, *Physical Review Letters* **117** (2016) 093003, *Scientific Reports* **6** (2016) 32653, or *Science* **354** (2016) 734

The objective of the project is to study attosecond and sub-femtosecond electron and nuclear dynamics in molecules 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 shall develop a research project on "Theoretical Attosecond Electron Dynamics", oriented to obtain a PhD diploma, to theoretically investigate the coupled electron and nuclear dynamics induced by attosecond laser pulses and strong electromagnetic fields on small and mid-size molecules, as well as in solids.

The successful applicant will perform novel theoretical developments and contribute to the implementation of highly parallelized computational tools, access vast technological resources through the European HP Computing Network, and will collaborate with top (theoretical and experimental) research groups in Atomic Molecular and Optical Physics across the world. Research stays and attendance to 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 which 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.

Related link to the position:
XChem European Research Council project: https://www.xchem.uam.es/xchem/