AttoChem COST Action Newsletter

Edition n.1, April 2020

In This Issue...

First ATTOCHEM WORKSHOP postponed to September

The 1st Annual Workshop of the COST Action CA18222 on Attosecond Chemistry has been postponed to September, 9-11, 2020. It will be held at the same location (Babeş-Bolyai University, Cluj-Napoca, Romania) and will be jointly organized with two parallel Working Group (WG1&WG2) meetings.

Follow us on LinkedIn and Twitter @ca18222!

Info on the Action's activities can be found on our webpage: https://attochem.qui.uam.es/.

CA18222 Action is supported by COST. COST is supported by the EU Framework Programme Horizon 2020. More information at CA18222.

CA18222 - Attosecond Chemistry

AttoChem Action is an **interdisciplinary network supported by COST**, whose main objective is to design new strategies for the control of charge migration in molecules by directly acting on the attosecond time scale. This ability will be used to selectively break and form chemical bonds, thus opening new avenues for the control of chemical reactions. **The AttoChem network will coordinate experimental and theoretical efforts to exploit the large potential of attosecond techniques in chemistry** and will also act as a liaison with the relevant stakeholders to bridge the gap to industrial applications.

Work Package 1

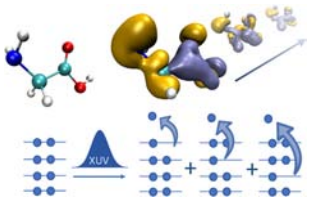
New attosecond techniques for the control of electron dynamics in molecules.

WG1 leader - Caterina Vozzi
caterina.vozzi@polimi.it

Work Package 2

Computational tools for the description of attosecond electron and nuclear dynamics.

WG2 leader - Ladislau Nagy
lnagy@phys.ubbcluj.ro



Work Package 3

Attosecond imaging and control of charge migration and chemical reactivity.

WG 3 - Franck Lepine
franck.lepine@univ-lyon1.fr

How to join the action?

If you want to join the Action you can register at our website following this link. Registration is per research group, namely only the group leader has to register by including information on other group members.

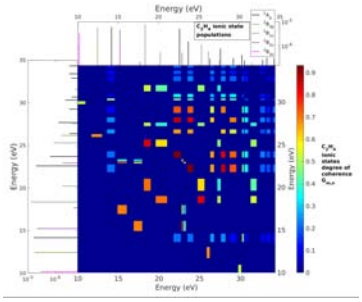
COST Action researchers win ERC Advanced Grants

- **Anne L'HUILLIER** (Lund University), for a project entitled ***Quantum Physics with Attosecond Pulses (QPAP)***. With the grant from ERC, Anne and colleagues plan to use laser technology to create ultra-short light pulses to study the motion of electrons within atoms and molecules.
- **Fernando MARTÍN** (Autonomous University of Madrid), for a project entitled: ***Imaging, Decoherence, and AttoSecond probing of ionization-induced charge migration in molecules (IDEAS)***. Its objective is to understand, and eventually predict, the first stages of charge migration processes in complex molecules, occurring in the time range of attoseconds.
- **Jonathan TENNYSON** (University College London), for a project entitled: ***Precision spectroscopic data for studies of exoplanets and other hot atmospheres (ExoMolHD)***. The project aims to provide data to enable astronomers to analyse the atmosphere of planets orbiting other stars, to better understand their composition.

The projects are among the 82 projects in the Physical Sciences and Engineering domain. **The sum of the three grants are bringing more than 7 million euros to carry out research**. For further information and details on these projects, follow this link.

Ultrafast charge dynamics in attosecond molecular ionisation

Marco Ruberti and Vitali Averbukh. The focus of their research is the study of fundamental ultrafast electronic processes occurring in atoms and molecules following excitation and/or ionization by ultrashort laser pulses. During the last few years, in collaboration with **Piero Decleva** (University of Trieste), they developed a disruptive theoretical methodology focused on the first principles description of ultrafast correlated many-electron dynamics in the presence of intense laser fields.



Degree of coherence between XUV-ionised states of C_2H_4. Part of 2019 PCCP HOT Articles [2].

The result of their work has been the first of its kind molecular ab initio method for many-electron wave packet dynamics in atoms and molecules, time-dependent B-spline ADC [1], which represents the **first successful attempt to adapt a traditional ab initio quantum chemical method to ionisation dynamics in real molecules**. The developed capability to model laser-induced many-electron processes from first principles is absolutely key to our ability to predict new physical phenomena as well as to guide the experimental science towards their observation and characterisation. **Contact:** V. Averbukh's group

1. V. Averbukh and M. Ruberti in *Attosecond Molecular Dynamics*, edited by M. Vrakking and F. Lepine, RSC Theoretical and Computational Chemistry series 13, 68 (2018).
2. M. Ruberti, Phys. Chem. Chem. Phys. 21, 17584 (2019), part of 2019 PCCP HOT Articles.

New collaboration

Marco Ruberti, Vitali Averbukh and the groups of Marc Vrakking and Misha Ivanov (MBI): development of the RCS-ADC approach [2] to characterize theoretically Raman-induced quantum electronic coherences in neutral molecules.

New funded project

Real-time Observation of Ultrafast Electron Motion using Attosecond XFEL Pulses, starting in December 2020. Experimental campaign led by the group of James P. Cryan, Agostino Marinelli and Peter Walter at the LCLS XFEL (Stanford), with Vitali Averbukh, Marco Ruberti, Fernando Martín, Alicia Palacios and Antonio Picon as theory collaborators.

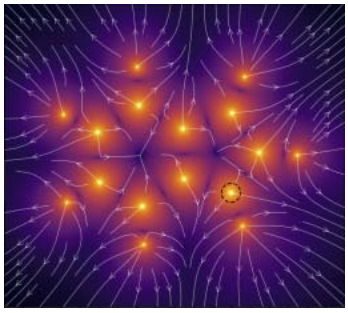
Software development

- Open source code YADE (https://yade-dem.org/doc/) is being developed by **Janek Kozick**. It has gained new boost multi-precision and just now quantum dynamics is implemented.
- **Patryk Jasik** is implementing and testing perturbation methods for precise assignment of diatomic spectra in his code named *Spyctroscopy*.
  Contact: Jozef Sienkiewicz's group
- UKRmol+: a suite for modelling electronic processes in molecules interacting with electrons, positrons and photons using the R-matrix method. The novel features of the code include the possibility to use B-splines for the description of the continuum and a new set of codes for photoionization calculations. The UKRmol+ codes constitute a major upgrade of the well-established UKRmol molecular R-matrix package for electron and positron scattering.
  See: https://doi.org/10.1016/j.cpc.2019.107092
- RMT: R-matrix with time-dependence. Solving the semi-relativistic, time-dependent Schrödinger equation for general, multielectron atoms and molecules in intense, ultrashort, arbitrarily polarized laser pulses. The RMT codes perform propagation of a multi-electron wavefunction in time using the R-matrix approach. See: https://doi.org/10.1016/j.cpc.2019.107062.
  Contact: Jimena Gorfinkiel's group

Jochen Küpper's group

A description of an advanced semiclassical model for electron dynamics in the combined strong laser and molecular field has been just submitted, preprint at here.

"Atomic-resolution imaging of carbonyl sulfide by laser-induced electron diffraction" was selected as **Editors' Choice 2019**, paper at here.



The quasistatic electric field exerted by the indole cation [Ref.].

PhD thesis

Evangelos Karamatskos defended his PhD thesis "*Molecular-Frame Angularly-Resolved Photoelectron Spectroscopy*" with destinctions. This work includes atomically resolved imaging of OCS molecules using strong-field ionization rescattering imaging, i.e., laser-induced electron diffraction.

Contact: Jochen Küpper's group

Andrej Mihelic's group

Work underway to enhance the recently developed theoretical approach used to calculate partial two- and multiphoton ionization amplitudes and cross sections [PRA 98, 023409 (2018)]. The approach avoids the use of a numerical extrapolation of the damping constant, which is employed in the time-independent exterior complex scaling calculations to limit the extent of the driving terms of the inhomogeneous Schrödinger equation.

Work on computer codes for solving the time-dependent Schrödinger equation for atoms with two active electrons which are driven by short intense laser pulses. The goal is to be able to accurately describe strongly coupled atomic continua.

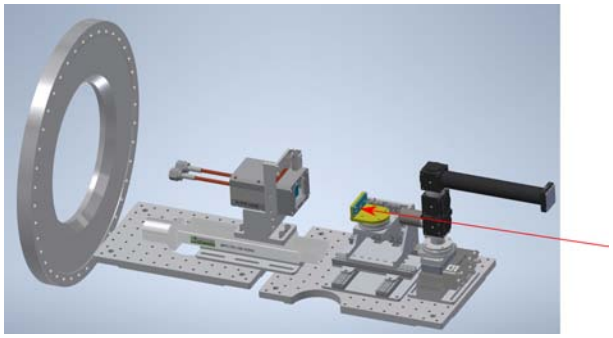
Contact: Andrej Mihelic's group

Violeta Petrović's group: Recent Submission of the manuscript entitled "*Tunneling Ionization Study of Linear Molecules in Strong-Field Laser Pulses*", V. Petrović, Hristina Delibašić and Ivan Petrović, for publication in Studia Physica, journal published by the Babeş-Bolyai University.

Contact: Violeta Petrović's group

Khakurel's group - ELI beamlines

ELI Beamlines is being developed as a centre of excellence for high power lasers and the secondary sources generated with them. Of the various types of secondary sources, the ones generating coherent flashes of EUV radiation is through **High Harmonic Generation**. A devoted beam-line and instrumentation has been constructed to perform AMO science and Coherent Diffraction Imaging. We look forward to collaborating with users willing to exploit our system and explore opportunities to perform static and time-resolved imaging experiments. **The technique and instruments around Coherent Diffractive Imaging with HHG based EUV source can immediately be translated to Attosecond-SpectroImaging which is in the common interest of the author and the action**.



A schematic for the coherent diffraction imaging of solid target at ELI beamlines. The red line indicates the direction of the EUV beam, which goes through an inline microscope and is incident on the sample. The diffraction pattern is recorded in the forward scattering geometry by a PI-MTE detector.

Contact: Krishna Khakurel's group

Software development

Anna Dzarasova's group

New version of QEC software 1.1 http://www.quantemol.com/qec-release-notes/

We also introduced new online features to the database of plasma chemistries: Global Model and Boltzmann Solver for plasma modellers. See: www.quantemolDB.co

Contact: Anna Dzarasova's group @quantemol on Twitter

QUANTUM BATTLES 2020

Virtual workshop focused on the quantum aspects of attoscience. Registration is free and it covers many topics of interest to the network. Visit Quantumbattles website www.quantumbattles.com or the Twitter page @quantumbattles.

Contact: Carla Figueira de Morisson Faria's group

Ultrafast Thin-Disk based CPA System with >.1kW Output Power and <.500 fs Pulse Duration

We demonstrated a very versatile Ytterbium thin-disk CPA system which can deliver a maximum output energy of 206 mJ at 5 kHz repetition rate with a pulse duration of 500 fs. Switching to 20 kHz repetition rate an output power of 1.95 kW (97.5 mJ at 800 fs) was reached. Further improvements will focus on increasing the pulse energy and pulse duration limit of this platform.

Contact: Thomas Metzger's group

SHORT TERM SCIENTIFIC MISSIONS (STSM)

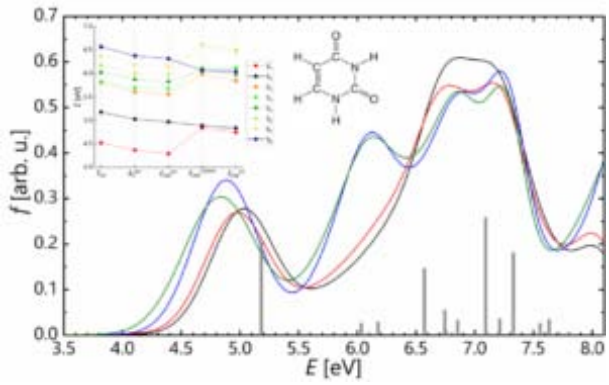
How to apply for a STSM

STSM applications must be submitted online using this e-cost platform. STSM applications are managed by the **STSM-Coordinator, Prof. Bernard Piraux** directly trough e-cost. STSM beneficiaries will be asked to provide a scientific report and a summary for outreach purposes after completion of the research mission. Failure to submit these reports within 30 days may effectively cancel the grant.

STSM RESULTS: Theoretical assignment of the electronic spectra of aqueous uracil and state specific analysis of solvation effects

Mr Branislav Milovanović Faculty of Physical Chemistry, University of Belgrade, Belgrade, RS
Host Institution: Institute Rudjer Bošković, Zagreb (HR)

Due to their biological relevance, DNA nucleobases excited state dynamics is extensively examined both experimentally and theoretically. Understanding competing photophysical mechanisms that can lead to and prevent light-inducted damage of the DNA nucleobases is of interest because of their widespread potential biological and/or technological applications. Determination of the character of large number of the excited electronic states is a challenging problem for nucleobases and other polyatomic molecules in general. Thus, resolving this problem is one step forward in understanding physical consequences underlying electronic excitation for these systems. Using previously developed procedure (PCCP) we are able to automatically determine character of the excited electronic states of nucleobase uracil both in gas phase and aqueous solution. (See complete report here).



Total effect of solvation on the computed UV absorption spectra for uracil.

Inclusivness Target Countries (ITC) Conference Grants (CG)

ITC-CG can support Early Career Investigators (ECI) and PhD students who wish to attend an international conference on the topic of the Action to present results related or obtained in the frame of the network. ITC-CG applications must be submitted online using e-cost tool. Applications are managed by the **ITC-CG Manager, Agnes Vibók** directly through e-cost.

The Action Grant Holder (GH) is the Universidad Autónoma de Madrid (ES). Any question related to Action funds can be addressed to:

The GH Scientific Representative: Fernando Martín, attochem@uam.es.

The GH Scientific Representative: Beatriz Martin Llorente, attochem.ghmanager@uam.es.

Action Management Structure

- Action Chair: Fernando Martín (ES)
- Action Vice-Chair: Francesca Calegari (IT)
- STSM Coordinator: Bernard Piraux (BE)
- Science Communications Manager (SCM): Aurora Ponzi (HR)
- CPC on Geographical Inclusiveness and ITC-CG Manager: Agnes Vibók (HU)
- CPC on Gender Balance: Violeta Petrović (RS)
- CPC on Early Career Investigators (ECI): Iva Brezinova (AT)
- Advisory Board: It is composed by L. Argenti (US), L. DiMauro (US), K. Ueda (JP), M. García (ES), T. Metzger (DE)

REMINDER!!!

Include the acknowledgement to COST/CA18222 Action on publications. Note that Action results have to be **co-authored by at least two Action participants** from two countries participating in the Action.

Editorial board: Aurora Ponzi