1st Training School of COST Action CM1204
XUV/X-ray light and fast ions for ultrafast chemistry (XLIC)

Module 2: New Computational Methods for Attosecond Molecular Processes

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MAIN FOCUS

The recent development of novel light sources like x-ray free-electron lasers and table-top lasers for high-harmonic generation, which are capable of delivering controllable sequences of intense subfemtosecond ionizing pulses, has opened the way to the monitoring and control of electron dynamics in atoms and molecules at its natural attosecond time scale. The coherent superpositions of highly excited states across a wide spectral range above the ionization threshold generated by the interaction of molecules with such pulses defeat the capabilities of most standard quantum-chemistry packages. In fact, the stationary state-based pictures familiar from lowest-order time-dependent perturbation theory may become altogether inapplicable.

The purpose of this school, organized in cooperation with the **XLIC COST Action CM1204**, is to introduce its participants to state-of-the-art ab-initio, hybrid and TDDFT numerical methods that can cope with ultra-fast dynamics, with an emphasis on unbound states in strong-fields and on the need to go beyond single-active-electron models to properly account for the role of correlation.

TOPICS

The tutorial will be organized in 5 theoretical sessions and 4 practical sessions in the computer lab. Both theoretical and practical sessions will be of 4 hours.

The school comprise four didactic blocks. The first block has an introductory character. It offers an overview of the field and a tutorial on strong field physics. The following three blocks focus on systems of increasing complexity and will be devoted to the description and use of new computational methods for fast time evolution in correlated systems in non-perturbative conditions (see description below). The school will end with a comprehensive overview of state-of-the-art results in attosecond pump-probe and strong field molecular science obtained with ab initio “exact” simulations in small systems, on the one side, and with TD-DFT effective-field simulations, capable of coping with larger systems, on the other side. The future perspectives, challenges and mutual interaction of these two complementary approaches will be discussed. The theoretical lectures will be complemented with 4 practical sessions.

THEORETICAL SESSIONS *(preliminary description – check for updates on the webpage of the school)*

1st Block [Ivanov, Smirnova]: Ionization in strong laser fields: Basic Theory, Analytical approximations, and physical picture.

2nd Block [Scrinzi]: Extreme ionization, static ionization rates and the breakdown of the "states" concept. Numerical and theoretical challenges associated to the description of strongly-driven electrons in the continuum, with the introduction of infinite-range Exterior Complex Scaling (ir-ECS) as a perfect absorber for time-dependent problems and the role of correlation in strongly-driven two-electron systems, with the introduction of the time-dependent surface-flux method (t-SURFF) for the spectral analysis of many-body time-dependent wave functions.

3rd Block [Patchkovskii]: Short overview of molecular electronic structure as obtained with quantum-chemistry programs; introduction to the GAMESS software. Description and comparison of computational techniques for strong-field ionization of molecules with correlated electrons: i) the molecular Ammosov-Delone-Krainov tunneling method (MO-ADK), ii) the time-dependent resolution in ionic states method (TD-RIS), and iii) the exterior-complex-scaling Möller-Plesset 2 method (ECS MP2).

4th Block [Argenti, Castro]: Part 1. *Ab-initio* calculation of attosecond transient absorption spectra. Part 2. Introduction to density-functional theories: ground state, and time-dependent density-functional theory; Application of TDDFT to nonlinear phenomena; Laser-matter interaction with TDDFT.

Closing Lectures [Martín, Rubio]: Seminars on state-of-the-art results of attosecond molecular processes with ab-initio and effective-field time-dependent methods.

PRACTICAL WORK *(preliminary description – check for updates on the webpage of the school)*

Practical session 1 [Ivanov, Smirnova, Morales, Patchkovskii]: Numerical solution of the time-dependent Schröedinger equation for a single active electron in the presence of strong ultra-short laser pulses; calculation of various observables.

Practical session 2 [Scrinzi, Zielinksi]: The loss of a state-based picture in strong-field dynamics: simulations with the ir-ECS method. Theoretical challenges and numerical solutions for the two-electron problem: simulations with the t-SURFF method.

Practical session 3 [Patchkovskii, Morales]: Preparation of molecular electronic states with GAMESS. Calculation of ionization rates for selected molecular orientations with the MO-ADK, the TD-RIS and the ECS-MP2 methods.

Practical session 4 [Castro, De Giovannini]: 1. Introduction to the fundamentals of the octopus code: ground state calculations (Hydrogen and Helium atoms). 2. Time-propagations: lasers. 3. Photo-dissociation: resonant vs. non-resonant frequencies. 4. Photo-emission from an atom.

ATTENDEES PROFILE

The course is directed to advanced master students, PhD students and young post-doctoral researchers in atomic and molecular physics, theoretical chemistry and applied mathematics, with an interest in developing new software for coherent control of electronic currents in systems with chemical interest. The number of trainees will be capped between 30 and 40, depending on the profiles of the applicants.

PROVISIONAL SCHEDULE