Fall School: Matter in Action!

16th–17th
November 2026

iMATUS Santiago de Compostela



ORGANIZERS AND SPONSORS





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2026 FALL SCHOOL MATTER IN ACTION!

WELCOME!

Dear Participant,

Welcome to the **2026 Fall School Matter in Action!** organized by **USC-iMATUS-IGFAE**, **GELUR**, **IMDEA Nanoscience-MATRIX**, **CLPU-Laserlab Spain**, and partially sponsored by **AUSE**. The School will run from **Monday November 16 to Tuesday November 17** as a satellite event of the **Ultrafast Science and Technology Spain (USTS) 2026** conference celebrated from **Wednesday November 18 to Friday November 20**.

The School venue is **Instituto de Materiales (iMATUS)**, belonging to the **University of Santiago de Compostela (USC)**, and which counts with the necessary conditions for the development of the School.

In the following you will find a description of the organization of the School, including the scientific program which includes **four scientific sessions** with lectures by the distinguished invited speakers and **short flash talks by the participants**.

We will do our best for you to have a satisfactory stay during the School at Santiago de Compostela.

We hope your participation will be scientifically rewarding and that you enjoy these days.

For comments or questions please contact us anytime.

The Organizing Committee
2026 Fall School Matter in Action!

VENUE

Instituto de Materiales (iMATUS)

The will be held at the Institute of Materials (iMATUS). The venue is located in the Campus Vida from the University of Santiago de Compostela (USC). The campus is within walking distance from the city center (but be aware of the Galician rain in November!).

Address:
Avenida do Mestre Mateo, 25
15706 Santiago de Compostela, Spain



SCIENTIFIC PROGRAM

The program is scheduled around **four scientific sessions** led by distinguished invited speakers. The School will feature a selected group of internationally recognized researchers presenting recent advances and emerging themes in high-resolution spectroscopy, astrochemistry, ultrafast dynamics, strong-field physics, reaction dynamics and molecular simulations.

The invited speakers include:

- **Majed Chergui** (Elettra Sincrotone Trieste, Italy & EPFL Lausanne, Switzerland)
- **Wojciech Gawelda** (Universität Paderborn, Germany)
- **Marcos Dantus** (Michigan State University, USA)
- **Fernando Martín** (IMDEA Nanoscience & Universidad Autónoma Madrid, Spain)

Each scientific session will extend for about two hours. In all cases the sessions will be divided in two parts.

The scientific sessions will be organized in **morning and afternoon sessions**, and will respect breaks for coffee and lunch times.

In addition to the scientific sessions, the students are welcome to participate in the school with a **flash talk presenting their doctoral or present research** (10 min including questions). These open sessions are designed to favor the communication between the participants and to exchange research experiences. The student presentations will be moderated by one of the invited speakers at the school.

We encourage all participants to engage actively in scientific discussions during both the invited talks and student talks.

The scientific program is included below. The student talks have been included in between the morning and afternoon sessions (Monday and Tuesday).

SCIENTIFIC PROGRAM

Monday 16 November 2026

9:00-11:00 **Majed Chergui** Elettra Sincrotone Trieste & EPFL Lausanne
Insights into Matter in Action using Ultrafast X-ray Spectroscopies

11:00-11:45 Coffee Break

11:45-13:35 **Flash presentations** by students (10 min including questions)

13:35-15:00 Lunch

15:00-17:00 **Wojciech Gawelda** Universität Paderborn
From Synchrotrons to XFELs: Element-Specific Probes of Structural Dynamics in Functional Molecules and Nanomaterials

17:00 - Free time

Tuesday 17 November 2026

9:00-11:00 **Marcos Dantus** Michigan State University
What Happens when an Energetic Electron (15-100 eV) Hits a Molecule?

11:00-11:45 Coffee Break

11:45-13:35 **Flash presentations** by students (10 min including questions)

13:35-15:00 Lunch

15:00-17:00 **Fernando Martín** IMDEA Nanoscience & UAM
Theoretical Attosecond Molecular Dynamics

17:00 - Free time

Insights into Matter in Action using ultrafast X-ray Spectroscopies

Majed Chergui

Elettra Sincrotrone Trieste, Strada Statale 14 - km 163,5 in AREA Science Park, 34149 Basovizza, Trieste, Italy
and
Lausanne Centre for Ultrafast Science (LACUS), ISIC, Faculté des Sciences de Base, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Keywords : X-ray absorption, X-ray emission, RIXS, non-linear X-ray phenomena, X-ray Free electron lasers, pump-probe

X-ray spectroscopies (absorption, emission, resonant inelastic X-ray scattering-RIXS) provide information about the electronic and spin structure of specific element and the molecular structure around them.[1] Implementing ultrafast X-ray spectroscopies allows one to therefore follow in real-time both the structural changes and the underlying electronic ones that drive them. Examples will demonstrate such capabilities on molecular systems in the condensed phase,[2] proteins[3] and solid materials.[4]
X-ray Free Electron lasers (XFEL) have emerged about 10 years ago as the source of choice for the above-mentioned studies. XFEL are also enabling non-linear X-ray spectroscopies,[5] much like the advent of the laser in the early 1960s brought about the birth of optical non-linear optics and spectroscopy. I will also present some of the achievements of X-ray non-linear spectroscopies and their unique ability to probe ultrafast phenomena with element-selectivity via hidden (to the optical domain) observables.

References

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(5) Chergui, M.; Beye, M.; Mukamel, S.; Svetina, C.; Masciovecchio, C. Progress and Prospects in Nonlinear Extreme-Ultraviolet and X-Ray Optics and Spectroscopy. *Nat. Rev. Phys.* **2023**, *5* (10), 578–596. https://doi.org/10.1038/s42254-023-00643-7

Learning objectives:

- Core advantages of X-ray spectroscopy: element-selectivity, structure sensitivity, electronic and spin structure
- Principles of time-resolved (pump-probe) spectroscopy using X-ray probes
- Applications of ultrafast optical pump/X-ray probe spectroscopy to (bio)molecular and condensed phase systems
- Principles of non-linear X-ray optics and its advantages: element-selectivity, high momentum transfers, nanometer resolution, observables hidden to linear spectroscopies
- Applications of ultrafast non-linear spectroscopies

From Synchrotrons to XFELs: Element-specific Probes of Structural Dynamics in Functional Molecules and Nanomaterials

Wojciech Gawelda

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Understanding how light triggers chemical transformations requires following electronic and nuclear rearrangements as they unfold over femtosecond-to-microsecond timescales. Time-resolved X-ray methods offer element-specific sensitivity to these coupled processes. Synchrotron facilities have enabled studies of transient structures with picosecond resolution, while X-ray free-electron lasers (XFELs) deliver intense, femtosecond X-ray pulses that can capture short-lived intermediates.

This tutorial will introduce the operating principles and complementary capabilities of synchrotrons and XFELs, explain the fundamentals of optical-pump/X-ray-probe experiments, and discuss how transient difference spectra can be related to changes in electronic and geometric structure. In particular, I will focus my attention to X-ray absorption spectroscopy (XAS), which is sensitive to oxidation states and local coordination environments, and X-ray emission spectroscopy (XES), which provides complementary information about metal-centered electronic and spin configurations. Connections to X-ray scattering and ultrafast optical spectroscopy will also be highlighted.

Representative examples will cover three classes of functional systems. First, transition-metal photosensitizers in homogeneous solution will illustrate how photoinduced electronic and geometric changes influence excited-state lifetimes, reductive quenching by sacrificial electron donors, and subsequent electron transfer to catalysts relevant to light-driven water splitting. Second, high-valent iron complexes will demonstrate how X-ray spectroscopy can characterize reactive intermediates relevant to biological and synthetic catalysis. Third, colloidal quantum dots will show how element-specific measurements can relate ultrafast charge-carrier dynamics to local structure and surface passivation in optoelectronic nanomaterials.

Throughout the lecture, the emphasis will be on connecting experimental observables with microscopic mechanisms. By combining complementary time-resolved probes, we can establish structure–function relationships and identify design principles for more efficient photocatalytic and optoelectronic materials.

References

[1] T. Katayama, *et al.*, *Chem. Sci.* **2023**, 14, 2572–2584
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[3] A. Burgos-Caminal *et al.*, *ACS Nano* **2025**, *19*, 21950–21961
[4] A. Burgos-Caminal *et al.*, *Chemistry of Materials* **2026**, *38*, 2601–2612

Learning objectives:

- learn basic principles of how accelerator-driven pulsed X-ray sources work (synchrotron and XFELs);
- understand fundamental concepts behind optical pump / X-ray probe experiments;
- learn how transient spectral differences can be related to both the electronic and geometric structure changes;
- identify different experimentally accessible observables using different X-ray spectroscopies or X-ray scattering methodologies and relate them to photoinduced physical or chemical processes in solvated molecules and colloidal nanoparticles.

What Happens When an Energetic Electron (15 – 100 eV) Hits a Molecule? Following the First Steps of Ionizing Radiation Chemistry

Marcos Dantus

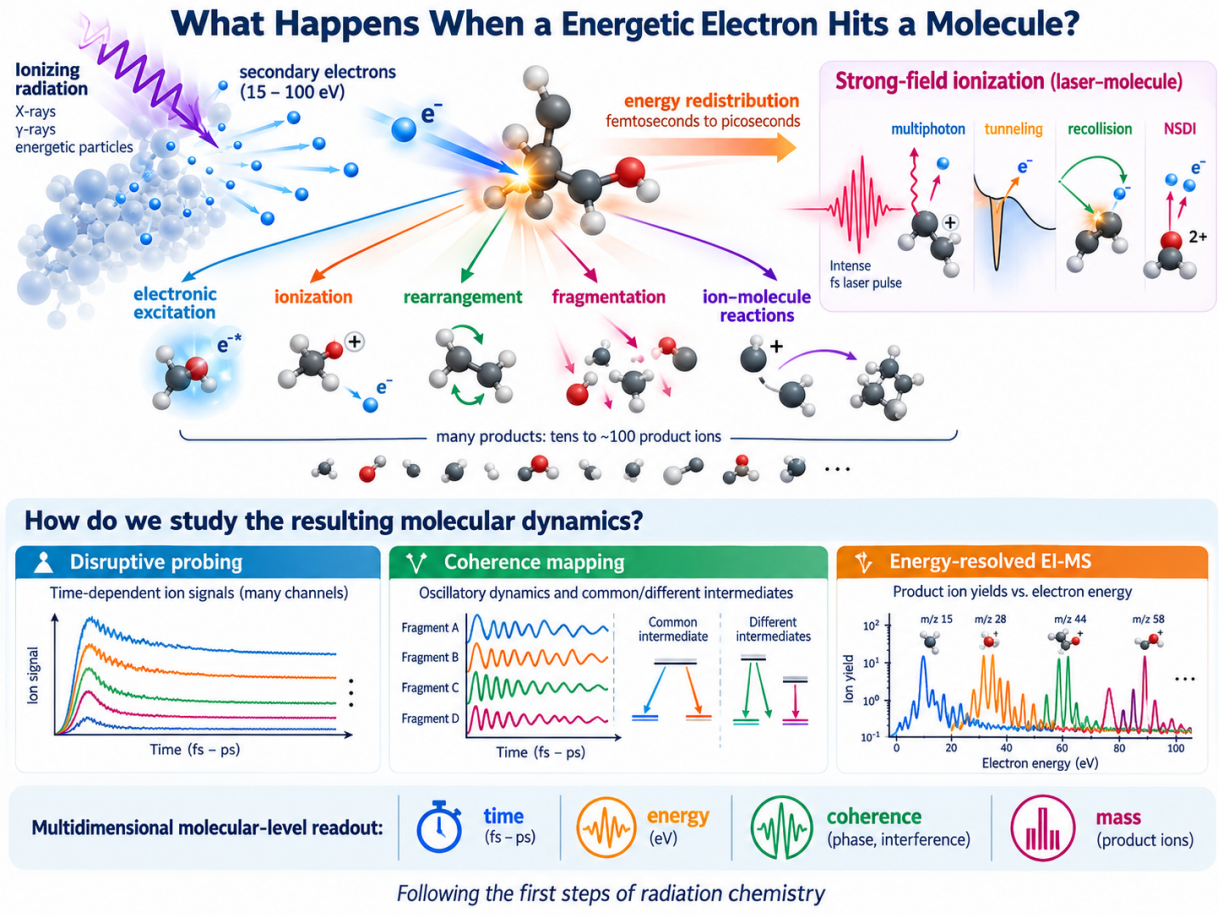
Department of Chemistry; Department of Electrical and Computer Engineering; Department of Physics and Astronomy; Michigan State University, East Lansing, MI, USA

Keywords: Ionizing radiation; radiation chemistry; secondary-electron chemistry; electron-impact ionization; molecular ion dynamics; fragmentation dynamics; ultrafast mass spectrometry; ion-molecule reactions.

Ionizing radiation deposits energy in matter in large part by generating energetic secondary electrons, and these electrons drive much of the ensuing molecular chemistry. When a 15–100 eV electron collides with a molecule, it can initiate electronic excitation, ionization, rearrangement, fragmentation, and subsequent ion-molecule reactions, opening a complex network of competing pathways [1]. How can we determine where the energy goes and reconstruct the dynamics when a single molecule can produce tens, or even nearly one hundred, different product ions? Disruptive probing allows many of these channels to be followed simultaneously [2], while coherence mapping can reveal whether different fragments arise through common or distinct dynamical intermediates [3]. Adding energy resolution provides a complementary dimension for unraveling dissociative ionization as it occurs in electron-ionization mass spectrometry [4]. Examples including H_3^+ formation [5], size-dependent proton transfer in methanol clusters [6], hydrogen-bond-directed chemistry, and ionic bimolecular reactions illustrate how time, energy, coherence, and mass can be combined to expose the molecular mechanisms initiated by energetic electrons. Strong-field ionization, from multiphoton and tunneling regimes through electron recollision and nonsequential double ionization, provides the ultrafast framework for accessing and probing many of these processes.

References

[1] M. Dantus, "Ultrafast studies of elusive chemical reactions in the gas phase," *Science* **385**, eadk1833 (2024). DOI: 10.1126/science.adk1833.
[2] B. Jochim, L. DeJesus, and M. Dantus, "Ultrafast disruptive probing: simultaneously keeping track of tens of reaction pathways," *Review of Scientific Instruments* **93**, 033003 (2022). DOI: 10.1063/5.0084837.
[3] J. Stamm et al., "Coherence mapping to identify the intermediates of multi-channel dissociative ionization," *Communications Chemistry* **7**, 103 (2024). DOI: 10.1038/s42004-024-01176-5.
[4] M. Dantus, "Tracking Molecular Fragmentation in Electron-Ionization Mass Spectrometry with Ultrafast Time Resolution," *Accounts of Chemical Research* **57** (2024). DOI: 10.1021/acs.accounts.3c00713.
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Following the first steps of radiation chemistry

Learning Objectives:

- Explain why secondary electrons generated by ionizing radiation are major drivers of molecular chemistry.
- Distinguish multiphoton ionization, tunnel ionization, electron recollision, and nonsequential double ionization.
- Describe how deposited energy is redistributed into electronic excitation, nuclear motion, fragmentation, rearrangement, and ion-molecule reactions.
- Explain how disruptive probing and coherence mapping reveal the time evolution and connections among many competing product channels.
- Describe how combining time, energy, coherence, and mass resolution helps unravel mechanisms of dissociative ionization.

Theoretical attosecond molecular dynamics

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Key Words: Ultrafast dynamics, attosecond chemistry, coherences and entanglement.

The advent of attoseconds light pulses (1 attosecond = 10^{-18} seconds), produced either in tabletop set ups or in kilometer-long X-ray free electron facilities, has opened the way to image and control electronic motion in atoms, molecules and solids at its natural time scale [1]. These tools are currently being used to follow in real time light-induced electron and charge transfer processes as those occurring in some of the most fundamental processes in nature, e.g., photooxidation, electronic transport and radiation damage. For this reason, attosecond light pulses are expected to have an important impact in physics and chemistry, as illustrated by the recently born field of Attosecond Chemistry [2,3]. The importance of the generation of attosecond pulses was recently recognized by the 2023 Nobel Prize in Physics awarded to Anne L'Huillier, Ferenc Krausz and Pierre Agostini, who, in their Nobel lecture, recognized the crucial role played by theoretical and computational investigations in their discovery and experimental characterization.
Describing the interaction of attosecond pulses with atoms and molecules goes beyond the capabilities of commercially available atomic-physics and quantum-chemistry computational approaches, as attosecond pulses are generated in the XUV and X-ray spectral ranges, thus leading to ionization of the system. For this reason, new theoretical methods and computational tools have been developed during the last decade (see, e.g., [4,5]). The goal of the school is to provide a solid theoretical basis and give access to the newly developed theoretical methods to describe electron and nuclear dynamics following ionization by attosecond pulses.

References

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[5] Special issue in Attosecond Chemistry software. *Computer Physics Communications* https://www.sciencedirect.com/special-issue/1066VSNVMGQ

Learning objectives

- To be aware of the main conceptual differences between electronic bound states and ionization (continuum) states in molecules as those populated by attosecond pulses.
- To be aware of the methods developed for the description of coupled electron and nuclear dynamics that follows the interaction with attosecond pulses.
- To learn how to associate measured attosecond time-resolved photoelectron and photo-ion spectra (the observables) with the actual attosecond dynamics taking place in molecules (the theoretical calculations).
- To identify the new directions in the field of attosecond molecular science for the coming years.

Flash presentations I
16 November 2026, 11:45-13:35

11:45-11:55	**Cintia Asensio Montejo**
11:55-12:05	**Marcos de Lucas Medina**
12:05-12:15	**Rodrigo González Fuentes**
12:15-12:25	**Aitana Hurtado Mendoza**
12:25-12:35	**Celtia Jabares Faraldo**
12:35-12:45	**Adhil Kabeer**
12:45-12:55	**Miguel Loureiro Muiños**
12:55-13:05	**Shahriar Mohammadi**
13:05-13:15	**Eva Otero Picón**

Flash presentations II
17 November 2026, 11:45-13:35

11:45-11:55	**Yago Radziunas Salinas**
11:55-12:05	**Sofía Rendo González**
12:05-12:15	**Judah Amir Renteria Lampaya**
12:15-12:25	**Judith Reyes**
12:25-12:35	**Marta Rodríguez Lorenzo**
12:35-12:45	**Alejandro Serrano Capote**
12:45-12:55	**Kushal Shaw**
12:55-13:05	**Belén Valiente Pascual**
13:05-13:15	**Iliana Hernández Cruz**

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