

COST Action CA20129
“Multiscale Irradiation and Chemistry
Driven Processes and Related Technologies”
(MultiChem)



Training School on
Multiscale computational and experimental
studies of irradiation-driven chemistry
processes

Instituto Superior Técnico
Lisbon, Portugal
October 03-07, 2022



Announcement

Scope

The 1st **Training School** of the [COST Action CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” \(MultiChem\)](#) will take place at the Instituto Superior Técnico (Lisbon, Portugal) during October 03-07, 2022.

The School is aimed to train the MultiChem Action’s participants (with a particular focus on Young Researchers and Investigators) in state-of-the-art theoretical, computational and experimental methods for studying the Irradiation-Driven Chemistry processes in (bio)molecular and nanoscale systems.

The 5-days-long School will be organized in the form of general lectures and hands-on practical tutorials. The lectures and tutorials will be given by experts in atomic and molecular physics, theoretical physics, physical chemistry, radiation physics and chemistry, and multiscale computational modeling. The School will also contribute to the networking activities of the COST Action and foster potential collaborations among the MultiChem participants.

The hands-on tutorials will be devoted to the exploration of physical models and computational approaches used for the simulations of Meso-Bio-Nano (MBN) systems and the investigation of their structure and dynamics at the atomic level of detail. In particular, the case studies of atomic & molecular clusters and nanoparticles; biomolecular systems; nanomaterials; composite materials and material interfaces; as well as dynamical, chemical, collision- and irradiation-driven multiscale phenomena will be discussed. Relevant physical concepts, mathematical techniques and computational methods will be introduced, including force fields and algorithms used in molecular modeling, molecular dynamics (classical, reactive and irradiation-driven) and stochastic dynamics simulations. The tutorials will be based on practical exercises with the advanced software packages [MBN Explorer](#) and [MBN Studio](#).

The Training School is designed for graduate students, postdoctoral researchers and staff in computational physics, chemistry and biology, molecular physics, radiation physics and chemistry, materials science, nanoscience, and radiobiology, who seek to extend their research skills to include theoretical, computational and experimental expertise, as well as for all other researchers interested in state-of-the-art methods for studying radiation-driven physics and chemistry processes.

Important Dates

Distribution of the announcement	June 17, 2022
Application open	June 17, 2022
Application deadline	July 15, 2022
Notification of acceptance	July 29, 2022

Call for applications

All the participants are requested to submit a registration form to team@mbnexplorer.com before July 15, 2022. Please indicate “*Application for the MultiChem training school*” in the email subject.

The registration form can be downloaded at the following webpage:
<https://mbnresearch.com/ca20129-multichem/training-schools/lisbon-2022-application>

Note that the number of training school participants is limited to 15.

Program¹

Monday, October 03

09 ³⁰ – 09 ⁴⁵	Training School opening
09 ⁴⁵ – 11 ⁰⁰	Multiscale modeling of irradiation-driven processes and phenomena (L)
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 12 ⁴⁵	Basics of MBN Explorer and MBN Studio and areas of application (L)
12 ⁴⁵ – 14 ⁰⁰	Lunch
14 ⁰⁰ – 15 ³⁰	Getting started/Setting up the calculations with MBN Explorer (T) Specification of input files and formats Introduction to MBN Studio (T) Overview of main features of MBN Studio; trial case studies representing certain physical experiments and demonstrating capacities of the program
15 ³⁰ – 16 ⁰⁰	Coffee break
16 ⁰⁰ – 18 ⁰⁰	Crystals, liquids, gases (T) Description of setting up simulations of gaseous, liquid and crystalline media with MBN Explorer; different types of boundary conditions; energy, temperature and pressure control in MBN Explorer Atomic and molecular clusters, nanoparticles (T) Construction of clusters and nanoparticles with MBN Studio; description of setting up calculations involving atomic clusters and nanoparticles

Tuesday, October 04

09 ³⁰ – 11 ⁰⁰	Biomolecular systems (T) Exploration of dynamical processes with biomolecular systems; use of the molecular mechanics potential for setting up calculations of biomolecular systems; simulation of bond breakage processes in biomolecular systems using MBN Explorer
11 ⁰⁰ – 11 ³⁰	Coffee break
13 ³⁰ – 13 ⁰⁰	Irradiation induced transformations of biomolecular systems (T) Exploration of dynamical processes related to the irradiation induced thermo-mechanical damage of molecular and biomolecular systems
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	Collision and irradiation induced processes (T) Molecular dynamics simulations of collision and irradiation-induced processes (fission, fusion, fragmentation) involving clusters, nanoparticles, as well as organic and inorganic molecular systems and materials
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	Reactive and Irradiation-Driven Molecular Dynamics (T) Introduction to the key principles of reactive molecular dynamics (RMD) and irradiation-driven molecular dynamics (IDMD) and related case studies

¹ L = Lectures, T = hands-on Tutorials

Wednesday, October 05

09 ³⁰ – 11 ⁰⁰	Nanostructured materials (T) Atomistic modeling of metallic, organic & inorganic nanomaterials and thin films. MD simulations of nanoscale phase and structural transitions
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	Thermomechanical properties of materials (T) Investigation of thermomechanical properties of crystalline, nanostructured and amorphous materials by means of MD simulations
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	Composite materials and material interfaces (T) Atomistic modeling of alloys and composites. MD simulations of deposition, diffusion and aggregation processes
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	Multiscale modeling using stochastic dynamics (T) Application of the stochastic dynamics method for simulations of fractal structures growth and their post-growth relaxation

Thursday, October 06

09 ³⁰ – 11 ⁰⁰	Collision physics: Electron collisions & Ion collisions (L) Understanding radiation damage of materials and radiotherapy requires an understanding of the interaction of different types of radiation with constituent atoms and molecules. Such collisions are defined by their cross section. In these lectures we will review basic collision processes and discuss the experimental methods by how collision cross sections are measured including the use of mass spectrometry.
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	Introduction to ion beam cancer therapy and related experiments (L) Ion beam Cancer Therapy (IBCT) has been highlighted as next generation radiotherapy technology. This session will review the principles, historical development, current status and current challenges of IBCT and describe several experiments that are directed towards understanding and developing IBCT.
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	Accelerator physics (L) Many radiotherapy techniques are based on the use of accelerators. This session will discuss accelerator design and operation with examples of their application in both the clinic for radiotherapy and in academic studies of materials.
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	Working at the nanoscale (L) Building structures at the nanoscale and the use of nanoparticles in medicine is at the forefront of modern technology and allowing new clinical treatments. In this session we will discuss how such nanosized objects are synthesized, characterized and imaged. Relevant experiments techniques such as TEM, AFM, STM, etc., will be reviewed.

Friday, October 07

09 ³⁰ – 11 ⁰⁰	A question of phase (L) This lecture will address the following questions: How do physical and chemical properties change as a function of phase? What are the experimental techniques used to study molecules in liquid and solid (condensed) phase?
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	Clusters – bridging the complexity gap (L) The study of molecular clusters provides a method of exploring how physical and chemical properties change from gaseous to solid phase. Recent experiments on clusters and their insight into radiation processes will be discussed.
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	Quantifying DNA damage (L) How do we measure damage to DNA and why is it important in assessing the dose that can be applied under clinical conditions? In this session we will discuss the methods used to observe and quantify radiation damage to DNA.
16 ⁰⁰ – 16 ¹⁵	Training School Closing

Venue and Travel Information

The Training School will take place at [Instituto Superior Técnico](#) (IST), Av. Rovisco Pais 1, 1049-001 Lisbon, Portugal.

To get to IST from the airport, take the red line of the metro and leave at Alameda station (16 min metro ride, 9 stations). See the travel map [here](#) for further details.

The ticket costs 1.50 € + 0.50 € for the card that you can always charge and use in all kinds of public transport in Lisbon. If you are using public transport just for airport transfer, buy 2 trips.



Accommodation

The organizers recommend the Training School attendees to book their accommodation in the following hotels located close to the venue. All the options are near IST and include breakfast. Participants are also advised to check prices at the hotel websites since sometimes they are cheaper there.

- 1) [Holiday Inn Lisbon](#), an IHG Hotel (2 min walking to IST)
- 2) [Hotel A.S. Lisboa](#) (5 min walking to IST)
- 3) [TURIM Alameda Hotel](#) (5 min walking to IST)
- 4) [Hotel Alif Campo Pequeno](#) (9 min walking to IST)
- 5) [Hotel ibis Lisboa Saldanha](#) (9 min walking to IST)

- 6) [Holiday Inn Express](#) - Lisbon - Plaza Saldanha, an IHG Hotel (9 min walking to IST)
- 7) [Le Premier Lisbon Suites](#) (10 min walking to IST)
- 8) [Empire Lisbon Hotel](#) (10 min walking to IST)
- 9) [VIP Executive Saldanha](#) (11 min walking to IST)
- 10) [Hotel Capital](#) (11 min walking to IST)
- 11) [Zenit Lisboa](#) (12 min walking to IST)
- 12) [Residencial Duque de Saldanha](#) (12 min walking to IST)
- 13) [Hills Hotel Lisboa](#) (15 min walking to IST)
- 14) [Chalet D'Ávila Guest House](#) (5 min walking to IST)
- 15) [Gaspar House](#) (11 min walking to IST)

Reimbursement of the travel expenses

The MultiChem COST Action provides financial support to reimburse training school participants for their travel expenses. Detailed information about the COST reimbursement rules can be found in the [Annotated Rules for COST Actions](#) (see Section 3.1 “Travel reimbursement rules”, pp. 82-88).

In order to be reimbursed you must receive an official invitation through e-COST indicating that you are eligible for the reimbursement. After the event, you will be required to fill in your online travel reimbursement request (OTRR) through the link you will find in the invitation email.

When arranging your travel and accommodation, please consider the following rules (see the Annotated Rules for COST Actions for complete and detailed information):

- Any transport you take in your country (airplane, train, bus, car...) is reimbursed based on the supporting documents provided (tickets for flights, trains and buses; proof of distance for car travel, e.g. by Google maps). Taxi, car rental, fuel and parking expenses are not eligible.
- For the flight ticket: it must be return and economy class ticket from the country of your primary affiliation (as registered in e-COST) to the country of the meeting. Seat reservation, luggage and cancellation insurance are eligible.

Official Invitation and Visa

Training school participants are advised to check the passport and visa requirements for travel to Portugal well in advance.

Sponsors

The Training School will be held under the auspices of the following sponsors:

- COST Action CA20129 MultiChem
- MBN Research Center gGmbH

List of Trainers

- Juraj Fedor (J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic)
- Nigel Mason (University of Kent, Canterbury, United Kingdom)
- Andrey Solov'yov (MBN Research Center, Frankfurt, Germany)
- Ilia Solov'yov (Carl von Ossietzky University, Oldenburg, Germany)
- Alexey Verkhovtsev (MBN Research Center, Frankfurt, Germany)

Training School Organizers

- Telma Marques (Instituto Superior Técnico, Lisbon, Portugal)
- Filipe Ferreira da Silva (Universidade NOVA de Lisboa, Caparica, Portugal)
- Alexey Verkhovtsev (MBN Research Center, Frankfurt, Germany)
- Juraj Fedor (J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic)
- Nigel Mason (University of Kent, Canterbury, United Kingdom)
- Andrey Solov'yov (MBN Research Center, Frankfurt, Germany)

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Up-to-date information on the Training School is available at the webpage:

<https://mbnresearch.com/ca20129-multichem/training-schools/lisbon-2022>

Relevant information on the MultiChem COST Action can be found at

<https://www.mbnresearch.com/ca20129-multichem/main>

<https://www.cost.eu/actions/CA20129/>

For any inquiries and for application submission, please write to team@mbnexplorer.com