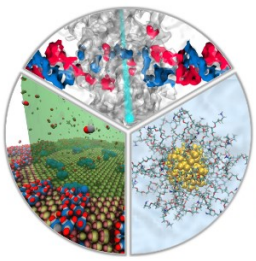


COST Action CA20129

MultIChem

Multiscale Irradiation and Chemistry Driven Processes and Related Technologies

cost

EUROPEAN COOPERATION IN SCIENCE & TECHNOLOGY

Training School on
Advanced computational methods and high-performance computing for MultIChem simulations

ATOMKI, Council Room
Debrecen, Hungary
March 28-30, 2023

Announcement

Scope

The **2nd Training School** of the COST Action CA20129 "Multiscale Irradiation and Chemistry Driven Processes and Related Technologies" (MultIChem) will take place at Atomki, the Institute for Nuclear Research of the Hungarian Academy of Sciences (Debrecen, Hungary) during March 28-30, 2023.

The Training School is aimed to train members of the MultIChem COST Action in state-of-the-art computational methods for multiscale simulations of Irradiation-Driven Chemistry processes involving (bio)molecular and nanoscale systems. The training will be delivered by experts in atomic and molecular physics, theoretical physics, physical chemistry, radiation physics and chemistry, multiscale computational modeling, and high-performance computing.

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, irradiation-driven, relativistic) 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	January 17, 2023
Application open	January 17, 2023
Application deadline	February 05, 2023
Notification of acceptance	February 12, 2023

Call for applications

All the participants are requested to submit a registration form to team@mbnexplorer.com before February 05, 2023. 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/debrecen-2023-application

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

Program

Tuesday, March 28

09^{30} – 09^{45}	**Training School opening**
09^{45} – 11^{00}	**Basics of MBN Explorer and MBN Studio and areas of application** Short description of main features of MBN Explorer and MBN Studio: universality, tunable force fields, multiscale approach, computational efficiency, etc. Areas of application of MBN Explorer and MBN Studio
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	**Setting up the calculations with MBN Explorer** Specification of input files and formats, and instructions on how to run the program **Introduction to MBN Studio** Overview of main features of MBN Studio. Trial case studies representing certain physical experiments and demonstrating capacities of the program
13^{00} – 14^{30}	**Lunch**
14^{30} – 16^{00}	**Crystals, liquids, gases, plasmas** 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
16^{00} – 16^{30}	**Coffee break**
16^{30} – 18^{00}	**Atomic and molecular clusters, nanoparticles** Construction of clusters and nanoparticles with MBN Studio. Description of setting up calculations involving atomic clusters and nanoparticles

Wednesday, March 29

09^{30} – 11^{00}	**Biomolecular systems** Exploration of dynamical processes with biomolecular systems using MBN Explorer. Use of the CHARMM molecular mechanics potential for setting up calculations of biomolecular systems. Reactive CHARMM (rCHARMM) potential and its application for the simulation of bond breakage processes in biomolecular systems
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	**Reactive Molecular Dynamics** Introduction to the key principles of reactive molecular dynamics (RMD) and related case studies. RMD simulations of collision-induced processes (fragmentation and association) involving clusters, nanoparticles, as well as organic and inorganic molecular systems and materials
13^{00} – 14^{30}	**Lunch**
14^{30} – 16^{00}	**Irradiation-Driven Molecular Dynamics** Introduction to the key principles of irradiation-driven molecular dynamics (IDMD) and related case studies
16^{00} – 16^{30}	**Coffee break**
16^{30} – 18^{00}	**Materials and interfaces (pt.1)** Computational design and investigation of structural and mechanical properties of materials (crystalline, amorphous, nanostructured) and their interfaces. Atomistic modeling of metallic, organic & inorganic nanomaterials and thin films. MD simulations of elastic and plastic deformations of materials.

Thursday, March 30

09^{30} – 11^{00}	**Materials and interfaces (pt.2)** Computational design and investigation of structural and mechanical properties of materials (crystalline, amorphous, nanostructured) and their interfaces. Atomistic modeling of metallic, organic & inorganic nanomaterials and thin films. MD simulations of elastic and plastic deformations of materials
11^{00} – 11^{30}	**Coffee break**
11^{30} – 13^{00}	**Thermomechanical properties of materials** Investigation of thermomechanical properties as well as phase and structural transitions of crystalline and nanostructured materials by means of MD simulations
13^{00} – 14^{30}	**Lunch**
14^{30} – 16^{00}	**Multiscale modeling using stochastic dynamics** Application of the stochastic dynamics method for simulations of fractal structures growth and their post-growth relaxation
16^{00} – 16^{30}	**Coffee break**
16^{30} – 18^{00}	**Relativistic dynamics of particles propagating through medium** Introduction to the key principles of relativistic molecular dynamics (RelMD). RelMD simulations of propagation of particles in various media, including linear and bent crystals, heterocrystalline structures, and amorphous materials
18^{00} – 18^{15}	**Training School closing**

Venue

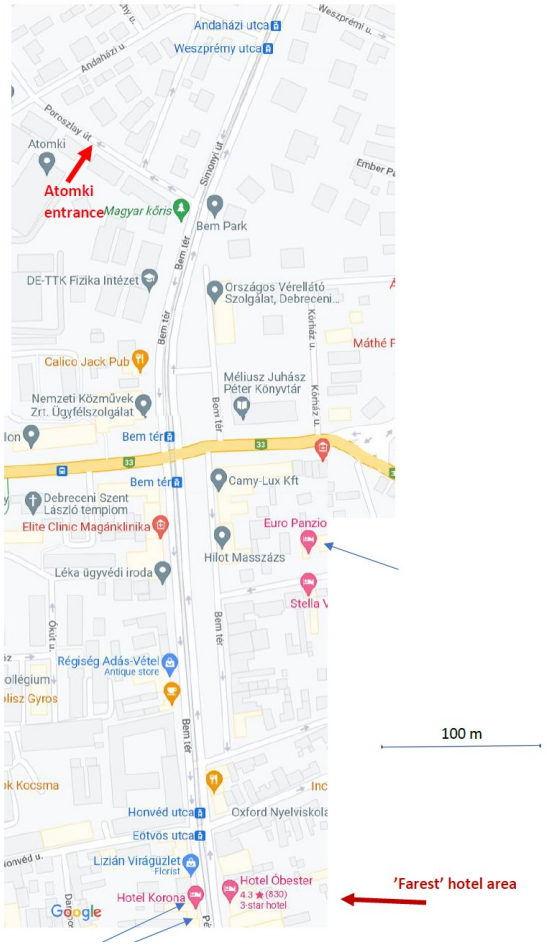
The Training School will take place in the Council Room of Atomki, the Institute for Nuclear Research of the Hungarian Academy of Sciences.

The address of the venue is:
Bem square 18/c, 4026 Debrecen, Hungary

Basic information about Atomki (including a brief description about how to get there) can be found on the following webpage:
https://www.atomki.hu/en/basic-information

The map on the right shows the surroundings of Atomki, several hotels located in the walking distance (5-8 min. walk) from the venue, and the stops of tram 1.

Additional information on the venue will be circulated closer to the beginning of the Training School.



Travel Information

Training School attendees are encouraged to explore a useful webpage about Debrecen (and how to get there) prepared for helping newcomer foreign students of the University: https://www.troubleshooter.hu/

Google map of Debrecen:
https://www.google.com/maps/place/Debrecen/@47.5321847,21.6122836,13z/?hl=en

If you arrive directly to Debrecen airport (https://www.debrecenairport.com/en), the best way is to take a taxi to a hotel or Atomki. Typical current costs are between 10-15 EUR.

Accommodation

The organizers recommend the Training School attendees to book their accommodation in the following hotels located in walking distance from the venue:

- Korona Panzió
  Address: Péterfia u. 54., 4026 Debrecen
  https://www.koronapanziodebrecen.hu/
  E-mail: info@koronapanziodebrecen.hu ,
  Telephone: +36 (52) 535-260

- Némethy Panzió
  Address: Péterfia u. 50, 4026 Debrecen
  http://www.nemethypanzio.hu/eng
  E-mail: info@nemethypanzio.hu
  Tel./Fax: +36 (52) 444-480

- Euro Panzió
  Address: Kétmalom u. 10, 4031 Debrecen
  http://www.europanzio.hu
  E-mail: info@europanzio.hu
  Phone (mobile): +36 30/417-4717

In all of these small hotels, a number of rooms have been reserved for the Training School attendees **up to March 15, 2023**.

For reservation, please contact the hotels directly by e-mail or phone, and indicate the keyword **"Atomki-MBN".**

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 A1-3.1 "Travel reimbursement rules", pp. 84-90).

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 Hungary 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

Training School Organizers

- Béla Sulik (Laboratory of Atomic and Molecular Physics, Atomki, Debrecen, Hungary)
- Alexey Verkhovtsev (MBN Research Center, Frankfurt, Germany)
- 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/debrecen-2023

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