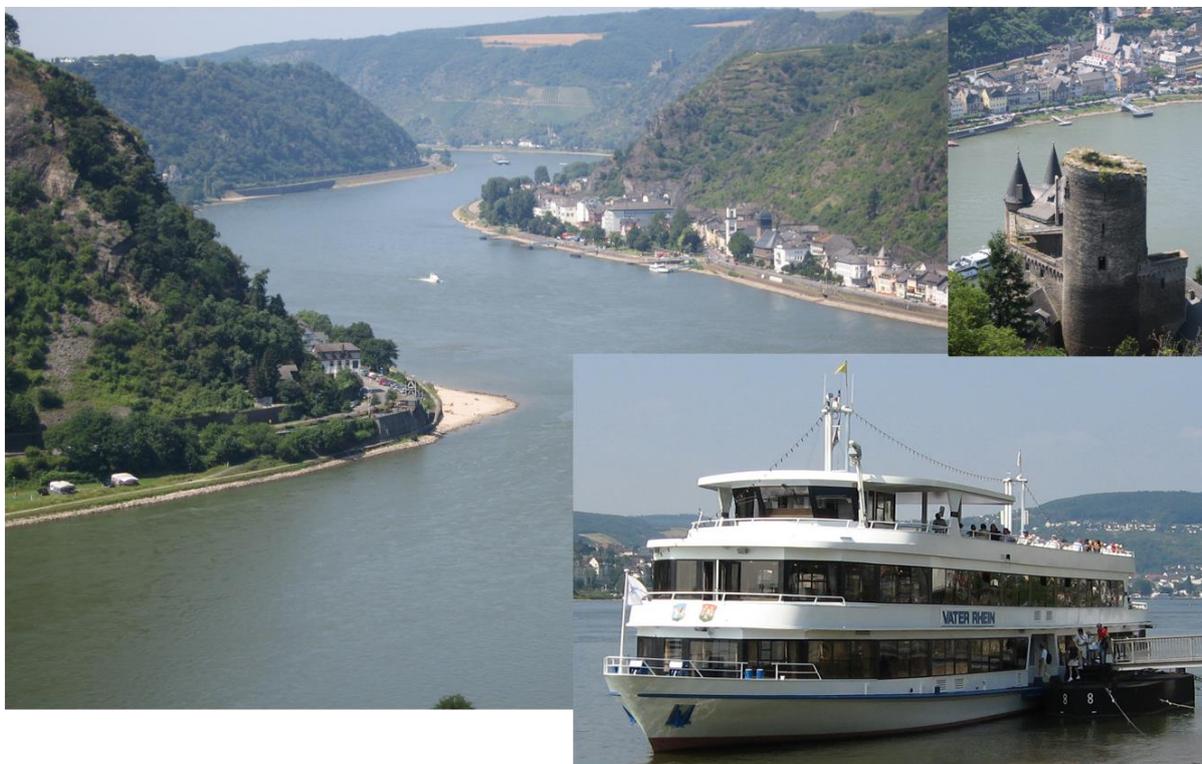


Multiscale Irradiation and Chemistry Driven Processes and Related Technologies

1st Annual MultiChem Conference (MultiChem 2022)

Stadthalle Boppard
Boppard am Rhein
Germany
May 16-18, 2022



Second Announcement

Scope

The 1st Annual Conference of the [COST Action CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” \(MultiChem 2022\)](#) will take place in Boppard am Rhein, Germany during May 16-18, 2022. The venue will be the Boppard city hall (Stadhalle Boppard).

The conference will bring together experts from different disciplines, such as physics, chemistry, biology, and materials science, specialized in the theoretical, multiscale computational modelling and experimental studies of irradiation-driven chemistry processes involving complex molecular systems exposed to radiation.

The scientific sessions will be followed by the MultiChem Management Committee meeting on May 18 to discuss further activities of the Action.

The following topics will be addressed within the MultiChem 2022 Conference:

- Collision and radiation processes involving nano- and biomolecular systems
- Radiation-induced chemistry
- Irradiation-driven transformations of molecular systems
- Biomedical and technological applications of radiation
- Related technologies: controlled nanofabrication with focused electron and ion beams, functionalized materials, nanocatalysis, etc.

Important Dates

Distribution of the first announcement	11.03.2022
Distribution of the second announcement	24.04.2022
Deadline for registration	30.04.2022
Deadline for abstract submission	30.04.2022

MultiChem 2022 scientific program

Monday, May 16

08 ⁰⁰ – 09 ¹⁵	Participants registration
09 ¹⁵ – 09 ³⁰	MultiChem 2022 Opening Alexey Verkhovtsev, Nigel Mason and Andrey Solov'yov
09 ³⁰ – 11 ⁰⁰	<u>Morning session I: Irradiation-driven transformations of molecular systems</u> Andrey Solov'yov , MBN Research Center, Frankfurt am Main, Germany <i>Multiscale modelling of irradiated MesoBioNano (MBN) systems with MBN Explorer and MBN Studio</i> Nigel Mason , University of Kent, Canterbury, United Kingdom <i>Experimental studies on radiation induced transformations of biomolecular systems and their application to radiotherapy</i> Pablo de Vera , University of Murcia, Murcia, Spain <i>The role of Monte Carlo simulations in multiscale modelling for biomedical and technological applications of radiation</i>
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<u>Morning session II: Radiation-induced chemistry</u> Gérard Baldacchino , Université Paris-Saclay, CEA, Gif-sur-Yvette, France <i>Huge dose rates in water can affect the initial equilibrium between ionization and excitation. Some expected consequences</i> Brendan Dromey , Queen's University Belfast, United Kingdom <i>Ultrafast Nanodosimetry - investigating the role of nanoscale structure and dynamics during radiation interactions in matter</i>

	Ilia Solov'yov , Carl von Ossietzky University of Oldenburg, Germany <i>Modelling of dynamical processes in molecular systems with stochastic dynamics</i>
13 ⁰⁰ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<u>Afternoon session I: Collision and radiation processes involving nano- and biomolecular systems</u> Thomas Schlathölder , Zernike Institute for Advanced Materials, University of Groningen, Netherlands <i>Gas-phase studies as a tool to investigate molecular mechanisms underlying radiation damage</i> Lorenzo Avaldi , Institute of Structure of Matter-CNR, Monterotondo, Italy <i>Unveiling inter- and intra-molecular interactions in homogeneous and hydrated uracil clusters by photoelectron spectroscopy</i> Amir Kotobi , Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany <i>Dynamic structure investigation and spectra prediction of peptides by machine learning techniques</i>
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	<u>Roadmap discussion</u> <u>Poster session</u>

Tuesday, May 17

9 ³⁰ – 11 ⁰⁰	<u>Morning session I: Irradiation-driven transformations of (bio)molecular systems and biological systems</u> Michael Hausmann , Kirchhoff-Institute for Physics, University of Heidelberg, Germany <i>Irradiation and biochemistry driven (re)organization of membrane receptors and cell nucleus chromatin domains</i> João Ameixa , University of Potsdam, Potsdam, Germany <i>DNA radiation damage studies using DNA origami nanostructures</i> Leo Sala , J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic <i>Ionizing radiation-induced damage to DNA in solution probed using DNA origami nanosupports</i>
11 ⁰⁰ – 11 ³⁰	Coffee break
11 ³⁰ – 13 ⁰⁰	<u>Morning session II: Biomedical and technological applications of radiation</u> Richard Amos , Department of Medical Physics and Biomedical Engineering, University College London, United Kingdom <i>Future directions in charged-particle radiotherapy: Opportunities and challenges</i> Dirk Wagenaar , University Medical Center Groningen, Netherlands <i>Radiobiological modelling in clinical treatment planning at the Groningen proton therapy center</i> Gohar Tsakanova , Institute of Molecular Biology NAS RA, Erevan, Armenia <i>Ultrashort pulsed electron beam irradiation: novel radiation modality for cancer treatment</i>
13 ⁰⁰ – 13 ¹⁵	Conference photo
13 ¹⁵ – 14 ³⁰	Lunch
14 ³⁰ – 16 ⁰⁰	<u>Afternoon session I: Nanofabrication with focused electron beams</u>

	<p>Harald Plank, Graz University of Technology, Graz, Austria <i>3D nanoprinting via focused electron beams: principles and applications</i></p> <p>Alexey Verkhovtsev, MBN Research Center, Frankfurt am Main, Germany <i>Atomistic simulations of irradiation-driven transformations involving organometallic systems</i></p> <p>Cornelis Hagen, Delft University of Technology, Delft, Netherland <i>Electron beam induced growth of hollow nano-cones: experiments and simulations</i></p>
16 ⁰⁰ – 16 ³⁰	Coffee break
16 ³⁰ – 18 ⁰⁰	<p>Afternoon session II: Irradiation-driven chemistry in FEBID and FIBID processes</p> <p>Lisa McElwee-White, Department of Chemistry, University of Florida <i>Custom precursors for FEBID/FIBID: comparison of electron- and ion-induced chemistry</i></p> <p>Sven Barth, Goethe University, Frankfurt am Main, Germany <i>Bimetallic precursors in focused particle-based deposition: FEBID vs. FIBID</i></p> <p>Iwona Szymańska, Nicolaus Copernicus University, Torun, Poland <i>Processes induced by electrons in molecules of coordination compounds</i></p>
19 ⁰⁰ – 22 ⁰⁰	Conference dinner

Wednesday, May 18

9 ⁰⁰ – 10 ³⁰	<p>Morning session I: Mechanisms of nanoparticle radiosensitization and catalysis</p> <p>Cécile Sicard-Roselli, Institut de Chimie Physique, University Paris Saclay, France <i>Do we need to decipher radiosensitization mechanism to consider biological applications?</i></p> <p>Olivier Tillement, NH TherAguix, France <i>Ultrasmall hybrid gadolinium-based nanoparticle as clinical radiosensitizer</i></p> <p>Theodoros Pavloudis, Nanomaterials Lab, University of Swansea, United Kingdom <i>Cluster-support interactions and their effect on the properties of Au nanostructures</i></p>
10 ³⁰ – 11 ⁰⁰	Coffee break
11 ⁰⁰ – 13 ⁰⁰	<p>Morning session II: Radiation-induced chemistry</p> <p>Juraj Fedor, J. Heyrovský Institute of Physical Chemistry, Czech Republic <i>Electron-induced chemistry: limits of single-collision-conditions data</i></p> <p>Duncan Mifsud, University of Kent, Canterbury, United Kingdom <i>Laboratory studies of astrochemical ices using mid-infrared spectroscopy</i></p> <p>Matija Zlataar, University of Belgrade, Serbia <i>Modeling metal-ligand bonds - from ground to excited states</i></p> <p>Malgorzata Smialek-Telega, Gdansk University of Technology, Gdansk, Poland <i>Cresols: the influence of the functional group positions</i></p>
13 ⁰⁰ – 13 ¹⁵	Final Discussion and MultiChem 2022 Closing
13 ¹⁵ – 14 ³⁰	Lunch
14 ³⁰ – 17 ⁰⁰	MultiChem Management Committee Meeting

Conference Venue and Travel Information

The conference will take place in Stadthalle Boppard (Boppard City Hall), Oberstraße 141, 56154 Boppard am Rhein, Germany.

Boppard is a small town located in a unique romantic Rhine Valley region, which has been declared a UNESCO World Heritage Site. There are more than forty castles stretched over an area

of 65 kilometers between Koblenz and Bingen along the riverbanks of the Rhine river and the famous Loreley rock, as well as a unique flora and fauna.

Boppard is located approximately 100 kilometers to the north-west from Frankfurt and 120 kilometers to the south from Cologne. You can get to Boppard by train from the Frankfurt Airport (<http://www.frankfurt-airport.com>) or Cologne/Bonn Airport (<https://www.cologne-bonn-airport.com/en/index.html>), or by car.

By train from:

- Frankfurt Airport (located about 100 km from Boppard), with flights to many cities in Europe. From the airport take either **(i)** a direct train (Regional Express, RE2) to Boppard (available on Monday morning, May 16) or **(ii)** a long-distance train (ICE) to Koblenz and change there to a regional train to Boppard (on Sunday, May 15). The travel will take approximately 2 hours.
- From Cologne/Bonn Airport take a train to Koblenz and change there to Boppard. The travel will also take approximately 2 hours.

The train schedule and tickets can be found at <http://www.bahn.de>

By car: take the exit 41-Boppard from the A61 Highway.

Registration

All the participants of the MultiChem conference are required to fill in an online registration form available at the following webpage:

<https://www.mbnresearch.com/1st-multichem-conference-2022-registration-form>

Please also check the actual information on the conference webpage:

<https://www.mbnresearch.com/ca20129-multichem/conferences/multichem-2022>

Registration Fee

The registration fee for the MultiChem 2022 Conference is **250 €**. The fee includes 3 lunches (on May 16, 17 & 18), coffee breaks, and the conference dinner (on May 17).

The payment to the order of “MultiChem 2022” should be made **by bank transfer** to

Bank Account Name:	MBN Research Center gGmbH
Bank name:	Deutsche Bank
Branch Address:	Hauptstr. 561462 Koenigstein Germany
IBAN:	DE15500700240137588000
BIC:	DEUTDEDBFRA

Please quote your **NAME** and **MultiChem** on the transfer.

If you need an invoice for the payment or want to pay with a credit card, please send a short email to team@mbnexplorer.com.

Accommodation

A limited number of rooms has been reserved for conference participants at the Bellevue Rheinhof, Rheinallee 41, 56154 Boppard am Rhein, Germany (<https://www.bellevue-boppard.de/en/>) with a discount price 125€ per person per night.

Please book your accommodation directly with the Hotel via e-mail: info@bellevue-boppard.de and quote “MultiChem”.



Reimbursement of the travel expenses

The MultiChem COST Action provides financial support to reimburse 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 meeting, 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.
- Your stay in Germany should be covered under the Daily Allowance (DA). The DA for Germany is 212€. The DA is intended to cover accommodation, meals and transport in the host country. No receipts will be required.
- The maximum DA rate that can be claimed is calculated according to the actual number of days you attend the meeting (as confirmed by your signature on the official attendance list for each day of the meeting), plus one day, permitting you to arrive on the day before the meeting and/or leave one day after.
- In the travel days, the DA is based on departure and arrival times (see p. 83 of the Annotated Rules for COST Actions).

Sponsors

The conference will be held under the auspices of the following sponsors:

- COST Action CA20129 MultiChem
- MBN Research Center gGmbH

Organizing Committee

- Alexey Verkhovtsev (MBN Research Center, Germany) - **Co-Chair**
- Nigel Mason (University of Kent, United Kingdom) - **Co-Chair**
- Andrey Solov'yov (MBN Research Center, Germany) - **Co-Chair**
- Irina Solovyeva (MBN Research Center, Germany)

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Updated information on the MultiChem 2022 Conference is available at the conference webpage <https://www.mbnresearch.com/ca20129-multichem/conferences/multichem-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 abstract submission, please write to team@mbnexplorer.com