



COST Action CA20129
MultIChem



The Second Conference
*" Multiscale Irradiation and Chemistry
Driven Processes and Related Technologies "*

MultIChem 2023

BOOK OF ABSTRACTS

Vila Lanna
Prague, Czech Republic
April 26-28, 2023

<https://www.jh-inst.cas.cz/multichem/>



Preface

Dear colleagues,

We welcome all participants to the 2nd conference of the COST Action CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” (MultiChem 2023). We are very pleased to host this meeting in Villa Lanna, a representative venue of the Czech Academy of Sciences in Prague.

MultiChem 2023 promises to be an exciting and stimulating conference with 30 oral and 30 poster presentations. It topically covers all areas that are of interest to the MultiChem COST action. At this meeting, in addition to academic partners, we have included contributions from industrial and clinical practice. The conference will also host the 2nd MultiChem Management Committee meeting which will happen in a hybrid in-person and online form.

We wish you a successful meeting and a pleasant stay in Prague!

Alexey Verkhovtsev
Juraj Fedor
(MultiChem 2023 chairs)

MultiChem Scientific Committee

- Alexey Verkhovtsev (MBN Research Center, Frankfurt am Main, Germany)
- Nigel Mason (University of Kent, Canterbury, UK)
- Andrey Solov'yov (MBN Research Center, Frankfurt am Main, Germany)
- Ilia Solov'yov (Carl von Ossietzky University, Oldenburg, Germany)
- Harald Plank (Graz University of Technology, Graz, Austria)
- Kate Ricketts (University College London, London, United Kingdom)
- Malgorzata Smialek-Telega (Gdansk University of Technology, Gdansk, Poland)
- Juraj Fedor (J. Heyrovský Institute of Physical Chemistry CAS, Czech Republic)

Organizing Committee

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- Alexey Verkhovtsev (MBN Research Center, Frankfurt am Main, Germany)
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Conference website

<https://www.jh-inst.cas.cz/multichem/>

Up-to-date information about the MultiChem 2023 conference and the COST Action MultiChem is available on the webpage <http://mbnresearch.com/ca20129-multichem/main>

Conference e-mail

multichem@jh-inst.cas.cz

General Information

Registration

The registration desk will be in the entrance hall of Villa Lanna on Wednesday, 26th April. In case of administrative questions, feel free to ask the organizers anytime during the conference.

Venue for Scientific Presentations

The talks will be given in the Apollo Hall, the main meeting room of Villa Lanna. Since we are approaching the capacity of the lecture room, we would like to ask you to also occupy places in the front rows, so that the rear seats are free for possible latecomers.

Poster Session

Poster session will be on Wednesday, 26th April at 18:00, in the entrance hall of Villa Lanna and in the back of the Apollo Hall. The poster panels will be set during the afternoon coffee break on Wednesday. The posters are not labeled, the participants are free to choose the panel according to their liking.

Conference Dinner

The conference dinner will be on Thursday, 27th April at 19:30, in the Restaurant and Brewery U Medvídků in the Old Town of Prague. The address of the restaurant is Na Perštýně 7. The dinner will be preceded by a beer tasting with a commentary from the brew master. The participants can get to the restaurant either by walking (3 to 5 km, depending on the chosen trajectory and on the amount of sightseeing) or by public transport. The fastest option is by green metro line A - start at station Hradčanská, exit at station Můstek. The local organizers will serve as guides for both of these options. Restaurant location may also be found by scanning the QR code or in the link below.



<https://goo.gl/maps/p5ry3kxR6W87X4iF8>

Management Committee meeting

The MC meeting will be on Friday, 28th April at 15:45. The meeting will take place in hybrid form in order to allow participation of MC members who do not attend the conference.

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Scientific Program

Wednesday, April 26

10 ⁰⁰ – 14 ⁰⁰	Participants registration
12 ³⁰ – 14 ⁰⁰	Lunch
14 ⁰⁰ – 14 ¹⁰	MultiChem 2023 Opening
	<u>Afternoon session I: Irradiation-driven transformations of molecular systems</u> (Chair: Alexey Verkhovtsev)
14 ¹⁰ – 14 ⁴⁰	Andrey Solov'yov , MBN Research Center, Frankfurt am Main, Germany <i>The fifth release of MBN Explorer and MBN Studio: Advances and challenges in multiscale computational modeling</i>
14 ⁴⁰ – 15 ¹⁰	Nigel Mason , University of Kent, Canterbury, United Kingdom <i>Solid state chemistry in astronomy – A new age</i>
15 ¹⁰ – 15 ⁴⁰	Brendan Dromey , Queen's University Belfast, United Kingdom <i>Narrow energy spread proton beams from a laser driven accelerator for high precision spatiotemporal measurements of ion damage in matter</i>
15 ⁴⁰ – 16 ⁰⁰	Coffee break
	<u>Afternoon session II: Electron interactions with nano- and biomolecular systems</u> (Chair: David Field)
16 ⁰⁰ – 16 ³⁰	Miloš Hrabovský , TESCAN, Czech Republic <i>Automation of FIB-SEM process and open-access control of nanopatterning</i>
16 ³⁰ – 17 ⁰⁰	Stefan Denifl , Institute for Ion Physics & Applied Physics, University of Innsbruck, Austria <i>Exploring reaction pathways of electron induced DNA damage</i>
17 ⁰⁰ – 17 ²⁰	Felipe Ferreira da Silva , Universidade NOVA de Lisboa, Caparica, Portugal <i>Electron interactions with astrochemical relevant molecules</i>
17 ²⁰ – 17 ⁴⁰	Mateusz Zawadzki , Gdansk University of Technology, Gdansk, Poland <i>Experimental studies on electron collisions with fundamental molecular targets</i>
17 ⁴⁰ – 19 ³⁰	Roadmap discussion (ca. 20-25 min) Poster session

Thursday, April 27

	<u>Morning session I: Ion interactions with biomolecular systems</u> (Chair: Hidetsugu Tsuchida)
09 ⁰⁰ – 09 ³⁰	Thomas Schlathölter , Zernike Institute for Advanced Materials, University of Groningen, the Netherlands <i>Heavy ion collisions with gas-phase DNA</i>
09 ³⁰ – 10 ⁰⁰	Alicja Domaracka , Centre de Recherche sur les Ions, les Matériaux et la Photonique, Normandie Université, Caen, France <i>Ions interacting with complex molecular systems: the effect of a surrounding environment</i>
09 ⁰⁰ – 10 ³⁰	Gérard Baldacchino , Université Paris-Saclay, France <i>What chemistry in the Bragg peak of protons and carbon ions?</i>
10 ³⁰ – 11 ⁰⁰	Coffee break

	<u>Morning session II: Irradiation-driven transformations of nano- and biomolecular systems</u> (Chair: Malgorzata Smialek-Telega)
11 ⁰⁰ – 11 ³⁰	Paola Bolognesi , CNR-Istituto di Struttura Della Materia, Monterotondo, Italy <i>Photoionisation studies of dipeptides</i>
11 ³⁰ – 12 ⁰⁰	Aleksandar Milosavljević , Synchrotron SOLEIL, Gif-Sur-Yvette, France <i>Near-edge x-ray absorption fine structure (NEXAFS) spectroscopy of protonated adenosine triphosphate molecule</i>
12 ⁰⁰ – 12 ³⁰	Alexey Verkhovtsev , MBN Research Center, Frankfurt am Main, Germany <i>Quantum mechanical inputs for irradiation-driven molecular dynamics</i>
12 ³⁰ – 14 ⁰⁰	Lunch
	<u>Afternoon session I: Irradiation-driven chemistry in nanofabrication processes</u> (Chair: Matija Zlatar)
14 ⁰⁰ – 14 ³⁰	Ilia Solov'yov , Institute of Physics, Carl von Ossietzky University Oldenburg, Germany <i>Stochastic dynamics simulation of the focused electron beam induced deposition process</i>
14 ³⁰ – 15 ⁰⁰	Petra Swiderek , Institute of Applied and Physical Chemistry, University of Bremen, Germany <i>Electron-driven chemistry of NH₃: New insights from molecular synthesis and fundamental processes of nanofabrication</i>
14 ⁰⁰ – 15 ³⁰	Anne Lafosse , Institute of Molecular Sciences of Orsay, Université Paris-Saclay, France <i>Quantifying non-thermal desorption from molecular ices - Comparative study of photon and electron irradiation in the valence- and core-shell energy ranges</i>
15 ³⁰ – 16 ⁰⁰	Coffee break
	<u>Afternoon session II: Nanofabrication with focused particle beams</u> (Chair: Felipe Fantuzzi)
16 ⁰⁰ – 16 ³⁰	Jose Maria De Teresa , University of Zaragoza, Spain <i>Metallic structures grown by focused ion beam decomposition of condensed precursor layers and of metallorganic films</i>
16 ³⁰ – 17 ⁰⁰	Lukas Seewald , Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology, Austria <i>Recent progress in functional nanofabrication via 3D Nanoprinting</i>
17 ⁰⁰ – 17 ³⁰	Lisa McElwee-White , University of Florida, USA <i>(η^3-allyl)Ru(CO)₃X Precursors: From FEBID to photoassisted area selective deposition</i>
19 ³⁰ – 22 ⁰⁰	Conference dinner: Restaurant & Brewery U Medvídků

Friday, April 28

	<u>Morning session I: Biomedical and technological applications of radiation</u> (Chair: Michael Hausmann)
09 ⁰⁰ – 09 ³⁰	Andrew Nisbet , Department of Medical Physics & Biomedical Engineering, University College London, United Kingdom <i>Current challenges and future developments in photon beam treatment planning</i>
09 ³⁰ – 10 ⁰⁰	Richard Amos , Translational Proton Therapy Physics, University College London, United Kingdom <i>Planning and delivery of ion beam cancer therapy: Limitations of contemporary clinical practice</i>
10 ⁰⁰ – 10 ³⁰	Revaz Shanidze , Kutaisi International University, Georgia <i>New hadron therapy center in Kutaisi, Georgia</i>
10 ³⁰ – 11 ⁰⁰	Alexander Gerbershagen , The University Medical Center Groningen (UMCG), Groningen, the Netherlands <i>UMCG - from radiobiology to treatment planning</i>
11 ⁰⁰ – 11 ²⁰	Coffee break
	<u>Morning session II: Mechanisms of nanoparticle radiosensitization</u> (Chair: Marc Benjamin Hahn)
11 ²⁰ – 11 ⁵⁰	Martin Falk , Institute of Biophysics, Czech Academy of Sciences, Brno, Czech Republic <i>Is there a simple explanation for metal nanoparticle-mediated cell radiosensitization?</i>
11 ⁵⁰ – 12 ²⁰	Olivier Tillement , NH TherAguix, France <i>Chelating bio-polymer for metal extraction: from concept to clinic</i>
12 ²⁰ – 12 ⁴⁵	Cécile Sicard-Roselli , University Paris Saclay, France <i>Do we always want nanoparticles to enhance radical production?</i>
12 ⁴⁵ – 13 ⁰⁰	Yasmine Sebti , University of Sorbonne, Paris, France <i>Hafnium oxide nanoparticles as computed tomography contrast agent</i>
13 ⁰⁰ – 14 ⁰⁰	Lunch
	<u>Afternoon session I: Radiation-induced chemistry</u> (Chair: Juraj Fedor)
14 ⁰⁰ – 14 ³⁰	Stanislav Kadlec , Eaton European Innovation Center, Czech Republic <i>Radiation-induced effects in power distribution industry - switching arcs, streamers and breakdown in low and medium voltage devices</i>
14 ³⁰ – 15 ⁰⁰	Tomáš Homola , Ropllass, Czech Republic <i>Atmospheric pressure plasma sources for rapid treatment of nano and bio surfaces</i>
15 ⁰⁰ – 15 ²⁰	Majdi Hochlaf , Université Gustave Eiffel, Champs-sur-Marne, France <i>Irradiation-driven formation of abiotic O₂ from SO₂</i>
15 ²⁰ – 15 ³⁰	MultIChem 2023 Closing
15 ³⁰ – 15 ⁴⁵	Coffee break
15 ⁴⁵ – 17 ⁰⁰	<u>MultIChem Management Committee Meeting</u>

Understanding the fate of electronically excited states by quantum chemical calculations

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The electronically excited states of transition metal complexes are classified into inter-configurational and intra-configurational metal-centered, ligand-centered, and charge transfer states. Different (de)localization of electron density in different types of excitations results in different geometry distortions. We use quantum mechanical calculations within the time-dependent density functional theory (TD-DFT) framework to describe and characterize the excited states of transition-metal complexes. From the shape of potential energy curves, we elucidate their fate.

Examples of our work on Pt(PF₃)₄, Cr(CO)₆, Fe(CO)₅, and Cr(bpy)₃³⁺ will illustrate the differences between the fate of different types of excited states. The main aim of our work is to get chemical insight and control of metal-ligand bonding.

Acknowledgments:

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