

COST Action CA20129
**“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



Conference 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
<u>09³⁰ – 11⁰⁰</u>	<u>Morning session I: Irradiation-driven transformations of molecular systems</u> (Chair: Alexey Verkhovtsev)
09 ³⁰ - 10 ⁰⁰	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>
10 ⁰⁰ - 10 ³⁰	Nigel Mason , University of Kent, Canterbury, United Kingdom <i>Experimental studies on radiation induced transformations of biomolecular systems and their application to radiotherapy</i>
10 ³⁰ - 11 ⁰⁰	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
<u>11³⁰ – 13⁰⁰</u>	<u>Morning session II: Radiation-induced chemistry</u> (Chair: Pablo de Vera)
11 ³⁰ - 12 ⁰⁰	G�rard Baldacchino , Universit� 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>
12 ⁰⁰ - 12 ³⁰	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>
12 ³⁰ - 13 ⁰⁰	Iia Solov'yov , Carl von Ossietzky University of Oldenburg, Oldenburg, Germany <i>Modelling of dynamical processes in molecular systems with stochastic dynamics</i>
13 ⁰⁰ – 14 ³⁰	Lunch
<u>14³⁰ – 16¹⁵</u>	<u>Afternoon session I: Collision, radiation and transport processes involving nano- and biomolecular systems</u> (Chair: Nigel Mason)
14 ³⁰ - 15 ⁰⁰	Thomas Schlath�lter , Zernike Institute for Advanced Materials, University of Groningen, Netherlands <i>Gas-phase studies as a tool to investigate molecular mechanisms underlying radiation damage</i>
15 ⁰⁰ - 15 ³⁰	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>
15 ³⁰ - 15 ⁵⁵	Theodoros Pavloudis , Nanomaterials Lab, University of Swansea, United Kingdom <i>Large-scale multi-method simulations in nanocluster science</i>
15 ⁵⁵ - 16 ¹⁵	Amir Kotobi , Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany <i>Dynamic structure investigation and spectra prediction of peptides by machine learning techniques</i>
16 ¹⁵ – 16 ⁴⁵	Coffee break
16 ⁴⁵ – 18 ⁰⁰	<u>Roadmap discussion & Poster session</u>

Tuesday, May 17

9³⁰ – 11⁰⁰	<u>Morning session I: Irradiation-driven transformations of (bio)molecular and biological systems</u> (Chair: Thomas Schlathölter)
09 ³⁰ - 10 ⁰⁰	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>
10 ⁰⁰ - 10 ³⁰	João Ameixa , University of Potsdam, Potsdam, Germany <i>DNA radiation damage studies using DNA origami nanostructures</i>
10 ³⁰ - 11 ⁰⁰	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>
11⁰⁰ – 11³⁰	Coffee break
11³⁰ – 13⁰⁰	<u>Morning session II: Biomedical and technological applications of radiation</u> (Chair: Andrey Solov'yov)
11 ³⁰ - 12 ⁰⁰	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>
12 ⁰⁰ - 12 ³⁰	Dirk Wagenaar , University Medical Center Groningen, the Netherlands <i>Radiobiological modelling in clinical treatment planning at the Groningen proton therapy center</i>
12 ³⁰ - 13 ⁰⁰	Gohar Tsakanova , Institute of Molecular Biology NAS RA, Erevan, Armenia <i>Ultrashort pulsed electron beam irradiation: novel radiation modality for cancer treatment</i>
13⁰⁰ – 13¹⁵	Conference photo
13¹⁵ – 14³⁰	Lunch
14³⁰ – 16⁰⁰	<u>Afternoon session I: Nanofabrication with focused electron beams</u> (Chair: Juraj Fedor)
14 ³⁰ - 15 ⁰⁰	Harald Plank , Graz University of Technology, Graz, Austria <i>3D nanoprinting via focused electron beams: principles and applications</i>
15 ⁰⁰ - 15 ³⁰	Alexey Verkhovtsev , MBN Research Center, Frankfurt am Main, Germany <i>Atomistic simulations of irradiation-driven transformations involving organometallic systems</i>
15 ³⁰ - 16 ⁰⁰	Cornelis Hagen , Delft University of Technology, Delft, Netherland <i>Electron beam induced growth of hollow nano-cones: experiments and simulations</i>
16⁰⁰ – 16³⁰	Coffee break
16³⁰ – 18¹⁵	<u>Afternoon session II: Irradiation-driven chemistry in FEBID and FIBID processes</u> (Chair: Harald Plank)
16 ³⁰ - 17 ⁰⁰	Lisa McElwee-White , Department of Chemistry, University of Florida <i>Custom precursors for FEBID/FIBID: comparison of electron- and ion-induced chemistry</i>
17 ⁰⁰ - 17 ³⁰	Sven Barth , Goethe University, Frankfurt am Main, Germany <i>Bimetallic precursors in focused particle-based deposition: FEBID vs. FIBID</i>
17 ³⁰ - 17 ⁵⁵	Iwona Szymańska , Nicolaus Copernicus University, Torun, Poland <i>Processes induced by electrons in molecules of coordination compounds</i>
17 ⁵⁵ - 18 ¹⁵	Cristiano Glessi , Delft University of Technology, Delft, Netherland <i>Fabrication of high purity platinum nanostructures through water-assisted simultaneous FEBID/FEBIE</i>
19¹⁵ – 22⁰⁰	Conference dinner

Wednesday, May 18

9⁰⁰ – 10³⁰	<u>Morning session I: Mechanisms of nanoparticle radiosensitization</u> (Chair: Malgorzata Smialek-Telega)
09 ⁰⁰ - 09 ³⁰	Cécile Sicard-Roselli , Institut de Chimie Physique, University Paris Saclay, France <i>Do we need to decipher radiosensitization mechanism to consider biological applications?</i>
09 ³⁰ - 10 ⁰⁰	Charnay Cunningham , Radiation Biophysics Division, iThemba LABS, National Research Foundation, Cape Town, South Africa <i>Radiosensitization effect of gold nanoparticles in proton therapy</i>
10 ⁰⁰ - 10 ³⁰	Olivier Tillement , NH TherAguix, France <i>Ultrasmall hybrid gadolinium-based nanoparticle as clinical radiosensitizer</i>
10³⁰ – 11⁰⁰	Coffee break
11⁰⁰ – 13⁰⁰	<u>Morning session II: Radiation-induced chemistry</u> (Chair: Iliia Solov'yov)
11 ⁰⁰ - 11 ³⁰	Juraj Fedor , J. Heyrovský Institute of Physical Chemistry, Czech Republic <i>Electron-induced chemistry: limits of single-collision-conditions data</i>
11 ³⁰ - 12 ⁰⁰	Duncan Mifsud , University of Kent, Canterbury, United Kingdom <i>Laboratory studies of astrochemical ices using mid-infrared spectroscopy</i>
12 ⁰⁰ - 12 ³⁰	Matija Zlatar , University of Belgrade, Serbia <i>Modeling metal-ligand bonds - from ground to excited states</i>
12 ³⁰ - 13 ⁰⁰	Malgorzata Smialek-Telega , Gdansk University of Technology, Gdansk, Poland <i>Cresols: the influence of the functional group positions</i>
13⁰⁰ – 13¹⁵	Final Discussion and MultiChem 2022 Closing
13¹⁵ – 14³⁰	Lunch
14³⁰ – 17⁰⁰	<u>MultiChem Management Committee Meeting</u>