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**
09^{30} – 11^{00}	**Morning session I: Irradiation-driven transformations of molecular systems** **(Chair: Alexey Verkhovtsev)**
09^{30} - 10^{00}	**Andrey Solov'yov**, MBN Research Center, Frankfurt am Main, Germany *Multiscale modelling of irradiated MesoBioNano (MBN) systems with MBN Explorer and MBN Studio*
10^{00} - 10^{30}	**Nigel Mason**, University of Kent, Canterbury, United Kingdom *Experimental studies on radiation induced transformations of biomolecular systems and their application to radiotherapy*
10^{30} - 11^{00}	**Pablo de Vera**, University of Murcia, Murcia, Spain *The role of Monte Carlo simulations in multiscale modelling for biomedical and technological applications of radiation*
11^{00} – 11^{30}	Coffee break
11^{30} – 13^{00}	**Morning session II: Radiation-induced chemistry** **(Chair: Pablo de Vera)**
11^{30} - 12^{00}	**Gérard Baldacchino**, Université Paris-Saclay, CEA, Gif-sur-Yvette, France *Huge dose rates in water can affect the initial equilibrium between ionization and excitation. Some expected consequences*
12^{00} - 12^{30}	**Brendan Dromey**, Queen's University Belfast, United Kingdom *Ultrafast Nanodosimetry - investigating the role of nanoscale structure and dynamics during radiation interactions in matter*
12^{30} - 13^{00}	**Ilia Solov'yov**, Carl von Ossietzky University of Oldenburg, Oldenburg, Germany *Modelling of dynamical processes in molecular systems with stochastic dynamics*
13^{00} – 14^{30}	Lunch
14^{30} – 16^{15}	**Afternoon session I: Collision, radiation and transport processes involving nano- and biomolecular systems** **(Chair: Nigel Mason)**
14^{30} - 15^{00}	**Thomas Schlathölter**, Zernike Institute for Advanced Materials, University of Groningen, Netherlands *Gas-phase studies as a tool to investigate molecular mechanisms underlying radiation damage*
15^{00} - 15^{30}	**Lorenzo Avaldi**, Institute of Structure of Matter-CNR, Monterotondo, Italy *Unveiling inter- and intra-molecular interactions in homogeneous and hydrated uracil clusters by photoelectron spectroscopy*
15^{30} - 15^{55}	**Theodoros Pavloudis**, Nanomaterials Lab, University of Swansea, United Kingdom *Large-scale multi-method simulations in nanocluster science*
15^{55} - 16^{15}	**Amir Kotobi**, Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany *Dynamic structure investigation and spectra prediction of peptides by machine learning techniques*
16^{15} – 16^{45}	Coffee break
16^{45} – 18^{00}	**Roadmap discussion & Poster session**

Tuesday, May 17

9^{30} – 11^{00}	**Morning session I: Irradiation-driven transformations of (bio)molecular and biological systems** **(Chair: Thomas Schlathölter)**
09^{30} - 10^{00}	**Michael Hausmann**, Kirchhoff-Institute for Physics, University of Heidelberg, Germany *Irradiation and biochemistry driven (re)organization of membrane receptors and cell nucleus chromatin domains*
10^{00} - 10^{30}	**João Ameixa**, University of Potsdam, Potsdam, Germany *DNA radiation damage studies using DNA origami nanostructures*
10^{30} - 11^{00}	**Leo Sala**, J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic *Ionizing radiation-induced damage to DNA in solution probed using DNA origami nanosupports*
11^{00} – 11^{30}	Coffee break
11^{30} – 13^{00}	**Morning session II: Biomedical and technological applications of radiation** **(Chair: Andrey Solov'yov)**
11^{30} - 12^{00}	**Richard Amos**, Department of Medical Physics and Biomedical Engineering, University College London, United Kingdom *Future directions in charged-particle radiotherapy: Opportunities and challenges*
12^{00} - 12^{30}	**Dirk Wagenaar**, University Medical Center Groningen, the Netherlands *Radiobiological modelling in clinical treatment planning at the Groningen proton therapy center*
12^{30} - 13^{00}	**Gohar Tsakanova**, Institute of Molecular Biology NAS RA, Erevan, Armenia *Ultrashort pulsed electron beam irradiation: novel radiation modality for cancer treatment*
13^{00} – 13^{15}	Conference photo
13^{15} – 14^{30}	Lunch
14^{30} – 16^{00}	**Afternoon session I: Nanofabrication with focused electron beams** **(Chair: Juraj Fedor)**
14^{30} - 15^{00}	**Harald Plank**, Graz University of Technology, Graz, Austria *3D nanoprinting via focused electron beams: principles and applications*
15^{00} - 15^{30}	**Alexey Verkhovtsev**, MBN Research Center, Frankfurt am Main, Germany *Atomistic simulations of irradiation-driven transformations involving organometallic systems*
15^{30} - 16^{00}	**Cornelis Hagen**, Delft University of Technology, Delft, Netherland *Electron beam induced growth of hollow nano-cones: experiments and simulations*
16^{00} – 16^{30}	Coffee break
16^{30} – 18^{15}	**Afternoon session II: Irradiation-driven chemistry in FEBID and FIBID processes** **(Chair: Harald Plank)**
16^{30} - 17^{00}	**Lisa McElwee-White**, Department of Chemistry, University of Florida *Custom precursors for FEBID/FIBID: comparison of electron- and ion-induced chemistry*
17^{00} - 17^{30}	**Sven Barth**, Goethe University, Frankfurt am Main, Germany *Bimetallic precursors in focused particle-based deposition: FEBID vs. FIBID*
17^{30} - 17^{55}	**Iwona Szymańska**, Nicolaus Copernicus University, Torun, Poland *Processes induced by electrons in molecules of coordination compounds*
17^{55} - 18^{15}	**Cristiano Glessi**, Delft University of Technology, Delft, Netherland *Fabrication of high purity platinum nanostructures through water-assisted simultaneous FEBID/FEBIE*
19^{15} – 22^{00}	Conference dinner

Wednesday, May 18

9^{00} – 10^{30}	**Morning session I: Mechanisms of nanoparticle radiosensitization** **(Chair: Malgorzata Smialek-Telega)**
09^{00} - 09^{30}	**Cécile Sicard-Roselli**, Institut de Chimie Physique, University Paris Saclay, France *Do we need to decipher radiosensitization mechanism to consider biological applications?*
09^{30} - 10^{00}	**Charnay Cunningham**, Radiation Biophysics Division, iThemba LABS, National Research Foundation, Cape Town, South Africa *Radiosensitization effect of gold nanoparticles in proton therapy*
10^{00} - 10^{30}	**Olivier Tillement**, NH TherAguix, France *Ultrasmall hybrid gadolinium-based nanoparticle as clinical radiosensitizer*
10^{30} – 11^{00}	Coffee break
11^{00} – 13^{00}	**Morning session II: Radiation-induced chemistry** **(Chair: Ilia Solov'yov)**
11^{00} - 11^{30}	**Juraj Fedor**, J. Heyrovský Institute of Physical Chemistry, Czech Republic *Electron-induced chemistry: limits of single-collision-conditions data*
11^{30} - 12^{00}	**Duncan Mifsud**, University of Kent, Canterbury, United Kingdom *Laboratory studies of astrochemical ices using mid-infrared spectroscopy*
12^{00} - 12^{30}	**Matija Zlatar**, University of Belgrade, Serbia *Modeling metal-ligand bonds - from ground to excited states*
12^{30} - 13^{00}	**Malgorzata Smialek-Telega**, Gdansk University of Technology, Gdansk, Poland *Cresols: the influence of the functional group positions*
13^{00} – 13^{15}	**Final Discussion and MultIChem 2022 Closing**
13^{15} – 14^{30}	Lunch
14^{30} – 17^{00}	**MultIChem Management Committee Meeting**

Modeling metal-ligand bonds – from ground to excited states

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The primary aspiration of modern chemistry is utilizing a single molecule to achieve the desired function. A fundamental understanding of all the factors affecting molecular properties is required to achieve this. All the properties of a molecule are inherently related to its electronic structure. In the case of a transition metal (TM) complex, the electronic structure is fundamentally guided by the number, geometry, and character (e.g., σ-donating or π*-back-donation, Fig. 1) of its metal-ligand bonds [1].

Significant theoretical efforts have been carried out in the last two decades to develop suitable methodologies to predict and rationalize the electronic structure of TM compounds. However, the matter remains open, and calculations on molecules with TM centers are still far from straightforward [2]. The main reason is that these calculations need a balanced treatment of both statical and dynamical correlation. Furthermore, it is necessary to understand the influences of coordination number, molecular symmetry, ligand-field strength, spin-orbit coupling, spin and oxidation states, redox potential, spin, and charge localization, electronic degeneracies, etc. [1-3]. Finally, a complete understanding of the electronic structure of TM compounds requires explorations that go beyond solely of ground states, i.e., consideration of excited states [1-4].

In this talk, our efforts in understanding and controlling metal-ligand bonding will be presented, mainly based on the density functional calculations. The influence of the excited states on the electronic ground state and the impact of the ground electronic state on the fate of excited states will be emphasized [4].

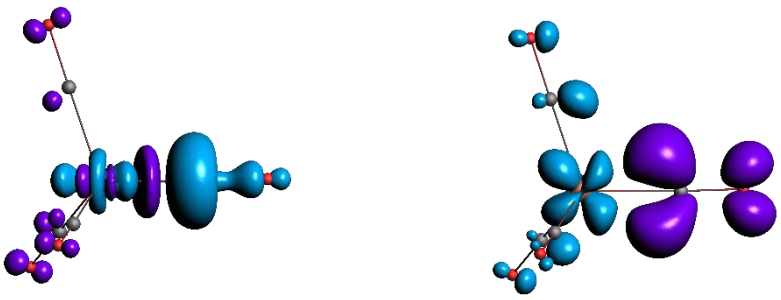

Figure 1: Example of Fe-CO σ- (left) and π- bonding (right) in $[Fe(CO)_4]^{2-}$ illustrated by density deformation channels; charge outfow/infow is represented by blue/purple color (electronic version) or light grey/dark grey (printed version), isovalue=0.005 a.u; see ref 2 for details.

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References:

[1] M. Zlatar, M. Gruden in *Practical Approaches to Biological Inorganic Chemistry, 2nd Edition*, 17 (**2020)**.
[2] M. Gruden, M. Zlatar, *Theoretical Chemistry Accounts*, **139**, 7, 126 (2020)
[3] C. Daul, M. Zlatar, M. Gruden-Pavlović, M. Swart in *Spin states in biochemistry and inorganic chemistry: influence on structure and reactivity*, 7 (2016)
[4] M. Zlatar, M. Allan, J. Fedor, *J. Phys. Chem. C*, **120** 10667 (2016)