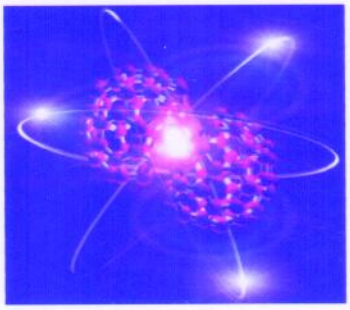
The 11th International Symposium
"Atomic Cluster Collisions"
ISACC 2023



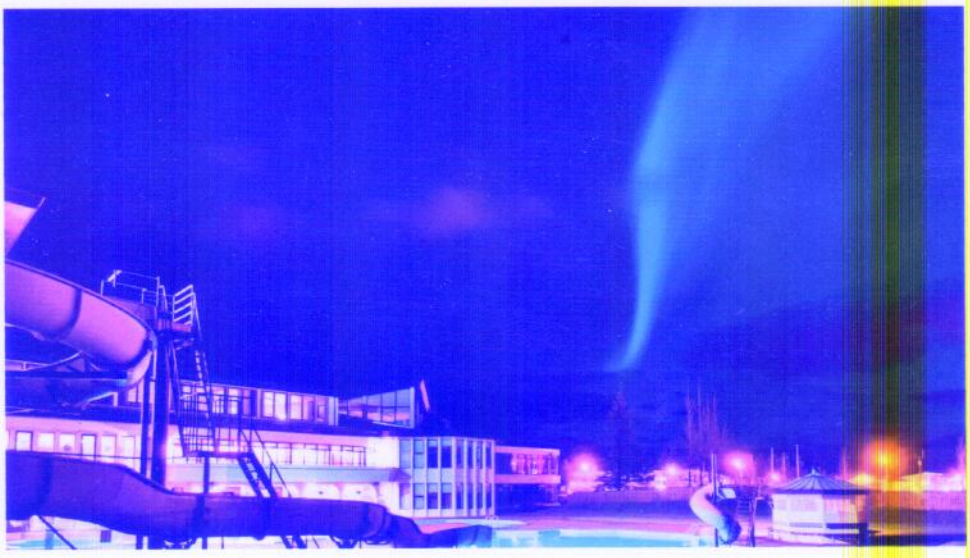
and

Workshop of the COST Action CA20129
"MultIChem"

COST Action CA20129
MultIChem

cost
EUROPEAN COOPERATION
IN SCIENCE & TECHNOLOGY

Hotel Örk
Hveragerði, Iceland
July 20-22, 2023



Book of Abstracts

Preface

The 11th International Symposium "Atomic Cluster Collisions" (ISACC 2023) and a thematically-related Workshop of the COST Action CA20129 "Multiscale Irradiation and Chemistry Driven Processes and Related Technologies" (MultIChem) will take place on **July 20-22, 2023** in Hveragerði, Iceland. The meeting is organized by MBN Research Center (Frankfurt am Main, Germany), Carl von Ossietzky University of Oldenburg (Oldenburg, Germany), and the University of Kent (Canterbury, United Kingdom).

A series of International Symposia "Atomic Cluster Collisions: structure and dynamics from the nuclear to the biological scale" started in 2003, and ten ISACC conferences have been held so far. The latest ISACC conference was organized in October 2021 jointly with the sixth International Conference "Dynamics of Systems on the Nanoscale" (DySoN) under the title "DySoN-ISACC 2021". Most of the ISACC conferences were satellites of the International Conferences on Photonic Electronic and Atomic Collisions (ICPEAC). The ISACC 2023 will be held just before the ICPEAC 2023 conference (Ottawa, Canada, July 25 – August 01, 2023).

The ISACC conference series promotes the growth and exchange of scientific information on the structure, properties and dynamics of complex nuclear, atomic, molecular, cluster, nanoscopic and biological systems studied primarily by means of photonic, electronic and atomic collisions. Particular attention is devoted to dynamical phenomena and many-body effects taking place in clusters, nanostructures, molecular and biological systems. These include problems of fusion and fission, fragmentation, collective electron excitations, phase transitions, radiation damage, and many more. Both experimental and theoretical aspects of cluster physics uniquely placed between nuclear physics on one hand and atomic, molecular and solid state physics on the other will be subject of the ISACC 2023 symposium. Particular attention at the Symposium will be devoted to the utilization of advanced computational techniques and high-performance computing for studying the aforementioned phenomena and effects. Links of the ISACC topics to novel and emerging technologies will be an important focus of the ISACC 2023.

Finally, ISACC 2023 will provide a platform to host discussions about current research and technological challenges and related initiatives within the ISACC Topical Areas.

Topical Areas of ISACC:

- Structure and dynamics of atomic clusters and nanoparticles
- Structure and dynamics of biomolecules and biomolecular clusters
- Reactivity and nanocatalysis
- Clustering in systems of various dimensionality and degrees of complexity
- Electron-, photon- and ion collisions with clusters and nanoparticles
- Electron-, photon- and ion collisions with biomolecules
- Complex collision, radiative and fragmentation processes
- Clusters and biomolecules in external (electric, magnetic, laser) fields
- Cluster and biomolecular research with Free Electron Lasers
- Related technological and medical applications

The **MultIChem Workshop** will focus on experimental, theoretical and computational modeling studies of irradiation- and chemistry driven multiscale phenomena. The focus will be made on the following research studies relevant to technological applications discussed within the MultIChem COST Action:

- Photon, electron and ion beam irradiation of isolated biomolecules in the gas phase
- Photon, electron and ion beam irradiation of molecular and biomolecular clusters
- Photon, electron and ion beam irradiation of deposited metal clusters and nanoparticles, and nanoparticles placed in a molecular environment.

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ISACC Conference Web Page

Updated information on the ISACC 2023 and the whole ISACC conference series is available at www.isacc-portal.org.

11th International Symposium *"Atomic Cluster Collisions"* (ISACC 2023)
and
Workshop of the COST Action CA20129 "MultIChem"

Hotel Örk, Hveragerði, Iceland, July 20-22, 2023

Thursday, July 20

10^{00} – 11^{15}	Participants registration
11^{15} – 11^{30}	**ISACC 2023 Opening**
11^{30} – 13^{00}	**Morning session I: Structural and phase transformations in nanoscopic systems** **(Chair: Shiv Khanna)** **Andrey Solov'yov**, MBN Research Center, Frankfurt am Main, Germany *On the mechanisms of radiation-induced structural transformations in metal clusters and biomolecules* **Florent Calvo**, University Grenoble Alpes / CNRS, Grenoble, France *Interplay between shape, size, and surface segregation in high-entropy nanoalloys* **Richard Palmer**, Nanomaterials Lab, Swansea University, Swansea, United Kingdom *Nanoclusters in the real world: Insights into deposited clusters from aberration-corrected electron microscopy*
13^{00} – 14^{30}	Lunch
14^{30} – 16^{00}	**Afternoon session I: Structure and dynamics of atomic clusters and nanoparticles** **(Chair: Florent Calvo)** **Hannes Jónsson**, Faculty of Physical Sciences, University of Iceland, Reykjavík, Iceland *Reassignment of 'magic numbers' for Au nanoclusters in the range of 50 to 2000 atoms* **Stefan Bergmeister**, Institute for Ion Physics and Applied Physics, University of Innsbruck, Austria *New developments in helium nanodroplet experiments* **Christoph Lienau**, Institute of Physics, Carl von Ossietzky University Oldenburg, Germany *Strong couplings in nanosystems: Manipulating transport properties by light*
16^{00} – 16^{30}	Coffee break
16^{30} – 17^{30}	**Afternoon session II: Reactivity and nanocatalysis** **(Chair: Richard Palmer)** **Shiv Khanna**, Physics Department, Virginia Commonwealth University, Richmond, USA *Ligated metal-chalcogenide clusters for nano p- n- junctions and for converting CO_2 to formic acid by tuning quantum states* **Jozef Lengyel**, TUM School of Natural Sciences, Technical University of Munich, Garching, Germany *Size effects in cluster chemistry and catalysis for the activation of small molecules*

Friday, July 21

09^{30} – 11^{00}	**Morning session I: Clusters and biomolecules in external fields** **(Chair: Himadri Chakraborty)** **John Sutter**, Science Division, Diamond Light Source Ltd, Chilton, United Kingdom *Diamond Light Source: the United Kingdom's synchrotron radiation facility* **Jan-Michael Rost**, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany *How does a fullerene dissipate its energy after multiphoton heating via the giant resonance?*

	Alexander Kuleff, Institute of Physical Chemistry, Heidelberg University, Germany *Ultrafast non-adiabatic relaxation in XUV-excited molecules: Dynamics in correlation bands*
11^{00} – 11^{30}	Coffee break
11^{30} – 13^{00}	**Morning session II: Collision and radiation-induced chemistry processes** **(Chair: Matija Zlatar)** **Nigel Mason**, School of Physics and Astronomy, University of Kent, Canterbury, UK *Clusters, aerosols and microdroplets – Complex chemistry revealed* **Filipe Ferreira da Silva**, Universidade NOVA de Lisboa, Caparica, Portugal *Boron complexes stability under electron interactions* **Anatoli Popov**, Institute of Solid State Physics, University of Latvia, Riga, Latvia *Distinctive features of point defect annealing in irradiated ceramic materials*
13^{00} – 14^{30}	Lunch
14^{30} – 16^{00}	**Afternoon session I: Electron-, photon- and ion collisions with biomolecular systems** **(Chair: Thomas Schlathölter)** **Ilia Solov'yov**, Institute of Physics, Carl von Ossietzky University Oldenburg, Germany *Modelling photoinduced electron transfers in complex molecular systems* **Franck Lépine**, Institut Lumière Matière, Université Claude Bernard Lyon 1, Villeurbanne, France *First instants following XUV ionization in complex (bio-)molecules: towards attosecond experiments in proteins and DNA* **Hidetsugu Tsuchida**, Quantum Science and Engineering Center, Kyoto University, Japan *Damage process of nucleotide molecules in water by ion irradiation*
16^{00} – 16^{30}	Lunch
16^{30} – 18^{00}	**Afternoon session II: Collision, radiative and fragmentation processes** **(Chair: Filipe Ferreira da Silva)** **Thomas Schlathölter**, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands *Implementation of a compact source for mass selected and conformationally pure biomolecular clusters* **Luca Gerhards**, Carl von Ossietzky University Oldenburg, Oldenburg, Germany *Modelling collision processes in complex molecular systems using VIKING* **Duncan Mifsud**, Institute for Nuclear Research (Atomki), Debrecen, Hungary *Intermolecular interactions in ice clusters: Relevance to radiation astrochemistry*
19^{00} – 22^{00}	Conference dinner

Saturday, July 22

09^{30} – 11^{00}	**Morning session I: Electron-, photon- and ion collisions with clusters and nanoparticles** **(Chair: Hannes Jónsson)** **Himadri Chakraborty**, Northwest Missouri State University, Maryville, USA *Femtosecond to attosecond electron dynamics in fullerene materials* **Jefferson Shinpaugh**, Department of Physics, East Carolina University, Greenville, USA *Nanostructured gold as a radiosensitizer for irradiation by ions* **Matthew Dickers**, School of Physics and Astronomy, University of Kent, Canterbury, UK *Atomistic modelling and structural characterisation of coated gold nanoparticles for biomedical applications*
11^{00} – 11^{30}	Coffee break

$11^{30} – 13^{00}$	**<u>Morning session II: Collision induced processes with organometallic molecules</u>** **(Chair: Nigel Mason)** **Alexey Verkhovtsev**, MBN Research Center, Frankfurt am Main, Germany *Irradiation-induced fragmentation of organometallic complexes studied by means of reactive molecular dynamics* **Matija Zlatar**, Department of Chemistry, University of Belgrade, Belgrade, Serbia *Quantum chemical insight into excited states of organometallic molecules* **Oddur Ingólfsson**, Science Institute and Department of Chemistry, University of Iceland, Reykjavík, Iceland *Low energy electron induced fragmentation and formation of gold containing deposits from $(CH_3)AuP(CH_3)_3$ and $[(CH_3)_2AuCl]_2$ by focused electron beam induced deposition*
$13^{00} – 14^{30}$	Lunch
$14^{30} – 16^{00}$	**<u>Afternoon session I: Collision, radiative and fragmentation processes</u>** **(Chair: Anatoli Popov)** **Józef Sienkiewicz**, Gdansk University of Technology, Gdansk, Poland *Optimization of the femtosecond laser impulse for excitation and the spin-orbit mediated dissociation in the NaRb dimer* **Alexander Karaivanov**, Faculty of Mathematics and Informatics, Sofia University, Bulgaria *CUDA Fortran implementation of Quantum Dissipative Dynamics code and its applications in stochastic descriptions of irradiation dynamics* **Alexander Platonenko**, Institute of Solid State Physics, University of Latvia, Riga, Latvia *Point defects diffusion in Al_2O_3 and $MgAl_2O_4$: ab initio study*
$16^{00} – 16^{10}$	**ISACC 2023 / MultIChem workshop Closing**

Quantum chemical insight into excited states of organometallic molecules

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Quantum chemical calculations are indispensable for characterizing and understanding a molecule's excited states. Excited states influence the spectroscopic, magnetic, and other properties of molecules. They also influence their reactivity. Therefore, understanding molecular excitations is of utmost importance.

In this talk, we will illustrate how different quantum chemical flavors are used in practice to deal with the excited states of organometallic and coordination compounds. We will show examples of the use of the time-dependent density functional theory (TD-DFT), ligand field DFT (LFDFT), the complete active space self-consistent field (CASSCF), and N-electron valence state perturbation theory (NEVPT2). We will address the benefits and shortcomings of these methods.

Acknowledgments:
This research was supported by the Science Fund of the Republic of Serbia, #7750288, Tailoring Molecular Magnets and Catalysts Based on Transition Metal Complexes – TMMagCat. The author thanks the Ministry of Science, Technological Development and Innovation of Republic of Serbia, Grant No. 451-03-47/2023-01/200026, and COST Action CA20129 MultIChem (Multiscale Irradiation and Chemistry Driven Processes and Related Technologies) for support.