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



and

Workshop of the COST Action CA20129 "MultIChem"





Hotel Örk Hveragerði, Iceland July 20-22, 2023

THIRD ANNOUNCEMENT

Scope

The 11th International Symposium <u>"Atomic Cluster Collisions"</u> (ISACC 2023) and a thematically-related Workshop of the <u>COST Action CA20129 "Multiscale Irradiation and Chemistry Driven Processes and Related Technologies"</u> (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 <u>held so far</u>. 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 <u>ICPEAC 2023</u> 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, 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
- 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 fields: electric, magnetic, laser etc.
- 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.

Scientific Program

Thursday, July 20

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$09^{00} - 11^{15}$	Participants registration			
$11^{15} - 11^{30}$	ISACC 2023 Opening			
$11^{30} - 13^{00}$	Morning session I: Structural and phase transformations in nanoscopic systems			
	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 Joseph Fourier, Grenoble, France Interplay between shape, size, and surface segregation in high-entropy nanoalloys			
	Richard Palmer, Swansea University, United Kingdom Nanoclusters in the real world			
$13^{00} - 14^{30}$	Lunch			
$14^{30} - 16^{00}$	Afternoon session I: Structure and dynamics of atomic clusters and nanoparticles			
	Hannes Jonsson, 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			
	Eric Suraud, Université Paul Sabatier, Toulouse, France On the stability of hole states in molecules and clusters, a generic mechanism?			
$16^{00} - 16^{30}$	Coffee break			
$16^{30} - 18^{00}$	Afternoon session II: Reactivity and nanocatalysis			
	Shiv Khanna , Virginia Commonwealth University, USA <i>Using superatomic metal-chalcogenide clusters and charge transfer ligands for nano p- n- junction with tunable band gaps and band alignment, light harvesting and CO₂ conversion</i>			
	Christoph Lienau, Carl von Ossietzky University Oldenburg, Germany Two-dimensional electronic spectroscopy: Probing strong couplings and charge transfer dynamics on the nanoscale			
	Jozef Lengyel, Department of Chemistry, Technical University of Munich 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					
	John Sutter, Diamond Light Source, 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					
	Ion spectra reveal spectra of neutral fragments ejected from fullerenes by FEL-XUV double pulses					
	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 processes					
	Nigel Mason , School of Physics and Astronomy, University of Kent, United Kingdom <i>Clusters, aerosols and microdroplets – Complex chemistry revealed</i>					

	Anatoli Popov , Institute of Solid State Physics, University of Latvia, Riga, Latvia Distinctive features of point defect annealing in irradiated ceramic materials			
	Fred Currell , Dalton Cumbrian Facility (DCF), University of Manchester, UK Modelling Inhomogeneous Radiation Chemistry using Linear Expansions (MIRaCLE), a promising approach			
$13^{00} - 14^{30}$	Lunch			
$14^{30} - 16^{00}$	Afternoon session I: Structure and dynamics of biomolecules Ilia Solov'yov, Carl von Ossietzky University Oldenburg, Germany Modelling photoinduced electron transfers in complex molecular systems			
	Thomas Schlatholter , Zernike Institute for Advanced Materials, University of Groningen, the Netherlands Implementation of a compact source for mass selected and conformationally pure biomolecular clusters			
	Bart Oostenrijk , Deutsches Elektronen-Synchrotron DESY, Hamburg, Germany Keeping it together: the stabilizing intra-peptide interaction between Sulphur and aromatic groups studied using VUV action spectroscopy			
$16^{00} - 16^{30}$	Coffee break			
$16^{30} - 18^{00}$	Afternoon session II: Electron-, photon- and ion collisions with molecular and biomolecular systems			
	Franck Lépine, Institut Lumière Matière, Université Lyon 1, France First instants following XUV ionization in complex (bio-)molecules: towards attosecond experiments in proteins and DNA			
	Hidetsugu Tsuchida, Kyoto University, Japan Damage of nucleotide molecules in liquid water caused by fast ion irradiation			
	Felipe Ferreira da Silva , Universidade NOVA de Lisboa, Caparica, Portugal Boron complexes stability under electron interactions			
$19^{00} - 22^{00}$	Conference dinner			

Saturday, July 22

$09^{30} - 11^{00}$	Morning session I: Electron-, photon- and ion collisions with clusters and nanoparticle				
	Himadri Chakraborty, Northwest Missouri State University, USA Femtosecond to attosecond electron dynamics in fullerene materials				
Jefferson Shinpaugh, East Carolina University, USA Radiosensitization properties of nanostructured gold and iron oxide (SPION) for irradions					
	Matthew Dickers, School of Physics and Astronomy, University of Kent, UK Atomistic modelling and structural characterisation of coated gold nanoparticles for biomedical applications				
$11^{00} - 11^{30}$	Coffee break				
$11^{30} - 13^{00}$	Morning session I: Collision induced processes with organometallic molecules				
	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, Serbia Quantum chemical insight into excited states of organometallic molecules				

	Oddur Ingolfsson, Department of Chemistry, University of Iceland, Reykjavik, Iceland Low energy electron induced fragmentation and formation of gold containing deposits from (CH ₃)AuP(CH ₃) ₃ and [(CH ₃) ₂ AuCl] ₂ by focused electron beam induced deposition			
$13^{00} - 14^{30}$	Lunch			
$14^{30} - 16^{30}$	Afternoon session I: Complex collision, radiative and fragmentation processes			
	Luca Gerhards, Carl von Ossietzky University 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			
	Alexander Karaivanov, Sofia University, Bulgaria / Université Paul Sabatier, Toulouse, France CUDA 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 <i>Point defects diffusion in Al</i> ₂ O_3 <i>and MgAl</i> ₂ O_4 : <i>ab initio study</i>			
$16^{30} - 16^{40}$	ISACC 2023 / MultIChem workshop Closing			

Registration

Late registration for the ISACC 2023 conference is still possible. The registration fee of 550 € includes access to the conference hall, coffee breaks, lunches, dinners on July 20 and 22, and the conference dinner on July 21.

The payment to the order of "ISACC 2023" 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 **ISACC2023** on the transfer. Please ensure there are NO charges to us.

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

Conference Venue

The Conference will be hosted by <u>Hotel Örk</u>, Breiðumörk 1c, 810 Hveragerði, Iceland.

The hotel is located in <u>Hveragerði</u>, one of Iceland's most popular destinations known as "The Hot Spring Town". The town known for its geothermal area with active hot springs is located in the south of Iceland, 45 km east (30 minutes) from the capital Reykjavík on Iceland's main ring road, Route 1.



Travel Information

From Keflavík International Airport to Reykjavík city center:

The <u>Keflavík International Airport</u> (KEF), which serves most international journeys to/from Iceland, is located approx. 50 km southwest of Reykjavík (see the map below). The Reykjavík city center (Bus Terminal BSÍ) can be reached from Keflavík Airport by buses operated by the companies <u>Strætó bs</u> and <u>Flybus</u>.

Strætó bs is a public transport company that operates city buses in Reykjavík and surrounding satellite towns and suburbs. Bus 55 from KEF to the Reykjavík city center operates according to the following schedule. The location of the Strætó bus stop at KEF is indicated on the following map.

The price for adults is 1.960 ISK (approx. 13 EUR). The duration of the bus trip is about 75 min.

Flybus operates in connection with all arriving flights at Keflavik Airport with direct transportation to Reykjavík City Center. Further information and the bus tickets can be found here. You can also buy tickets for the Flybus in vending machines at Keflavík Airport.

The price for adults is approx. 26 EUR. The duration of the bus trip is 45-50 min.

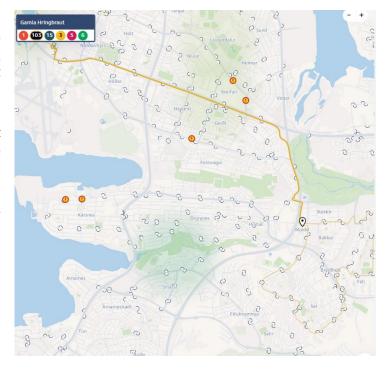


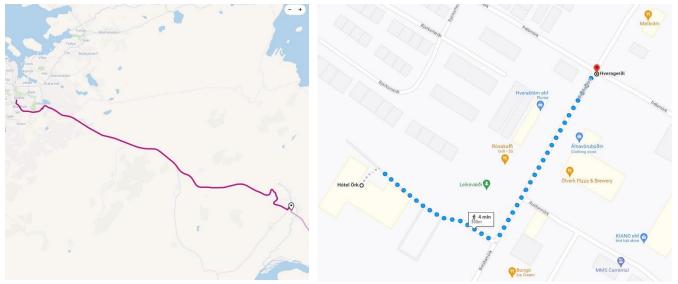
From Reykjavík city center to Hveragerði:

Take *Bus 3* (yellow route on the map to the right) in the direction Sel/Fell from the bus stop "Gamla Hringbraut" in the city center (2 min walk from the Bus Terminal BSÍ) and get off at the bus stop "Mjódd" (17 min ride; 7 stops).

There, change to *Bus 51* (purple route on the map below) in the direction of Selfoss and get off at the bus stop "Hveragerði" (37 min ride; 4 stops).

The conference venue, Hotel Örk, is within a 5 minutes walking distance from the Hveragerði bus stop.





Further information about this trip, including the route planner and bus timetables, can be found on the <u>Strætó website</u> (English version is available).

Accommodation

The participants should contact directly the conference venue Hotel Örk (<u>booking@hotelork.is</u>) regarding the accommodation.

Accommodation includes breakfast as well as access to a swimming pool, hot tubs, steam, and wireless internet. When booking accommodation, please quote "MBN23" to book one of the following rooms:

Room type	e No. of people staying Price per night		r night
		Icelandic Krónas (ISK)	EUR
Superior (27 m ²)	1	25.291	170
	2	36.285	244
	3/4	41.785	281

Further information on other types of rooms available at the hotel can be found <u>here</u>.

Abstract Submission

Abstracts should be submitted electronically **not later than June 15, 2023**. Please send your abstracts to <u>isacc.conference@gmail.com</u> with the title "ISACC 2023 Abstract".

The abstracts are to be supplied by the authors typewritten in camera-ready form in A4 format. The length of the abstract should not exceed two pages. The abstract template with more detailed preparation guidelines is available for downloading here.

Please note that we accept files in the MS Word document (.docx) format.

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- Alexey Verkhovtsev (MBN Research Center, Germany)

Sponsors

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

- MBN Research Center, Frankfurt am Main, Germany
- H2020-MSCA-RISE Project "RADON"

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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.

Conference e-mail

isacc.conference@gmail.com