

The 2024 Collisions Physics and Chemistry and their Applications Conference

and

A Workshop of the COST Action 20129: *Multiscale Irradiation and Chemistry Driven Processes and Related Technologies*

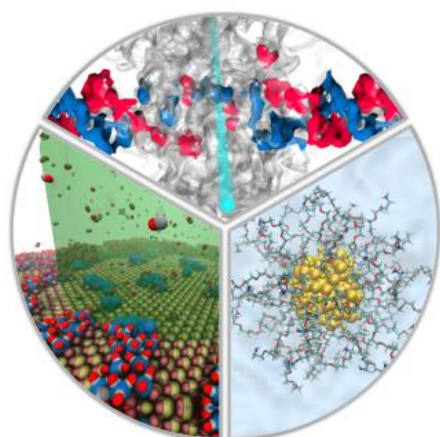
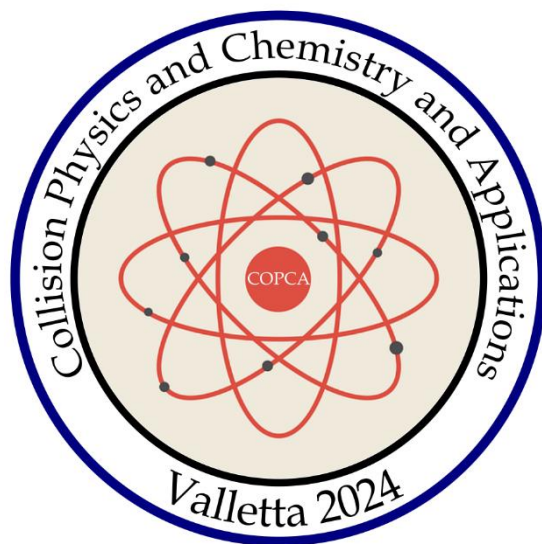


COPCA-MultIChem 2024

15th – 18th October 2024

Aula Magna, University of Malta, Valletta, Malta

ABSTRACT BOOKLET



COST Action CA20129

MultIChem

Multiscale Irradiation and Chemistry Driven
Processes and Related Technologies

CONFERENCE VENUE

The conference will be held in the Aula Magna at the Valletta campus of the University of Malta (Maltese: L-Università ta' Malta). The University was initially founded as the *Collegium Melitense* by the Jesuit Order in 1592, at a time when Malta was governed by the Knights Hospitaller of St John's of Jerusalem, Rhodes, and Malta (nowadays known as the Sovereign Military Order of Malta). The Old University Building, which houses the Aula Magna, was built by 1597.

Following the expulsion of the Jesuits from Malta in 1768, the college was taken over by the Knights Hospitaller and was elevated to full University status in 1769, when Grand Master Manuel Pinto da Fonseca signed a decree constituting a public university. The university was briefly suspending during the reign of Grand Master Francisco Ximénez de Tejada in the 1770s, but was quickly reconstituted by his successor Grand Master Emmanuel de Rohan-Polduc in 1779.

During the Napoleonic invasion and occupation of Malta between 1798-1800, the University was replaced by the *École Centrale*. The University was once again reopened under British rule in the early nineteenth century and, indeed, operated under the name of the Royal University of Malta until 1974, when the Maltese Monarchy was abolished and replaced by a republic. Nowadays, most of the University's lecturing and academic activities take place at the University campus in Msida, while the Valletta Campus is mainly used to host international conferences and seminars, along with a number of summer schools. It also currently houses the Research, Innovation and Development Trust (RIDT).



Valletta is the European Union's most southerly and smallest capital city. With a population of just over five thousand, it is also one of the smaller settlements in Malta. The city was built by the Knights Hospitaller starting in 1566 with the aim of increasing the defensibility of the island. This was motivated by the failed Ottoman invasion of Malta in 1565, in which two and a half thousand knights and militiamen defeated an Ottoman invasion force numbering forty thousand. The city was named in honour of the victorious Grand Master Jean Parisot de la Valette. The construction of the city was largely completed by the early 1570s, although its namesake did not live to see its completion: Grand Master de la Valette had died of a stroke in 1568. His successor, Grand Master Pietro del Monte, designated Valletta as Malta's capital city in 1571.

Valletta still serves as the Maltese capital city to this day, and is home to the Maltese parliament (although the President's official residence at the Palace of San Anton is located in the town of Attard, some six kilometres away). The city was officially designated as a UNESCO World Heritage site in 1980, and was recognised as the European Capital of Culture in 2018. Home to over three hundred monuments in an area of only half a square kilometre, Valletta is one of the most concentrated historic cities in the world.



CONFERENCE DINNER

The conference dinner will be held during the evening of Thursday, 17th October 2024 at the Trattoria AD1530 in the old fortified city of Mdina.

Established in the eighth century BC, Mdina served as Malta's former capital from antiquity up to the mediaeval period. The city is presently home to fewer than three hundred inhabitants, but was once the major settlement on the island, particularly during the Romano-Punic era. Following a massacre in the ninth century, the area was largely abandoned until its re-founding in the eleventh century by Islamic settlers from the Emirate of Sicily. The city's relative importance declined upon the arrival of the Knights Hospitaller in 1530, as they elected to make use of the city of Birgu as their capital. Although experiencing something of a revival in the early eighteenth century, during which time several Baroque-style buildings were erected, Mdina never regained its pre-1530 strategic or political importance; earning it the nickname *The Silent City*. Nowadays, Mdina is on the tentative list of UNESCO World Heritage Sites and is a popular tourist attraction.



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CONFERENCE WEBPAGE

The conference webpage may be found at: <https://copcaconference.wixsite.com/copca2024>

CONFERENCE PROGRAMME

Tuesday, 15th October 2024

Conference Day One (MultiChem Sessions)

- 09.00 Registration at Conference Venue
- 09.30 Opening Remarks: The COPCA Conference Series
Duncan V. Mifsud (HUN-REN Institute for Nuclear Research, Hungary)
- 09.45 Open Remarks: Multiscale Irradiation and Chemistry-Driven Processes and Related Technologies
Alexey V. Verkhovtsev (MBN Research Centre, Germany)
- Session 1: Modelling as a Tool for Understanding Multiscale Chemical Systems and Irradiation-Driven Processes**
Chair: Juraj Országh (Comenius University Bratislava, Slovakia)
- 10.00 Progress in Multiscale Computational Modelling of Meso-Bio-Nano Systems Exposed to Radiation
Andrey V. Solov'yov (MBN Research Centre, Germany)
- 10.30 Applications of Multiscale Modelling in Astrochemistry and Nanofabrication
Felipe Fantuzzi (University of Kent, United Kingdom)
- 11.00 Understanding the Spin States in Coordination Complexes
Matija Zlatar (University of Belgrade, Serbia)
- 11.30 **Coffee Break**
- 12.00 Modelling Collision Processes in Complex Molecular Systems Using VIKING
Ilia A. Solov'yov (University of Oldenburg, Germany)
- 12.30 Radiation-Induced Phenomena in Molecules and Atomic Clusters Studied with MBN Explorer and MBN Studio
Alexey V. Verkhovtsev (MBN Research Centre, Germany)
- 13:00 **Lunch Break**
- Session 2: Applications of High-Energy Science: Synchrotrons and Plasma**
Chair: Alexey V. Verkhovtsev (MBN Research Centre, Germany)

14.00 Atmospheric Pressure Low-Temperature Plasma for Application in Agriculture and Food Processing

Veronika Medvecká (Comenius University Bratislava, Slovakia)

14.30 Exploring Electrical Breakdown in Ultra-Low Global Warming Potential Gases for Insulation in Medium and High-Voltage Technology

Dragana Marić (Institute of Physics Belgrade, Serbia)

15.00 Computational Studies of Redox-Active Transition Metal Compounds

Furio Corà (University College London, United Kingdom)

15.30 Advancing the Performance of Li-Ion Batteries Using X-Rays

Maria Alfredsson (University of Kent, United Kingdom)

16.00 **Coffee Break**

Session 3: Early Career Researcher Presentations

Chair: Rebekah Attard-Trevisan (University of Kent, United Kingdom)

Presentation 1: Formation of Polyynes in 1 keV Electron Irradiated Interstellar Ice Analogues

Lars Borchert (University of Aarhus, Denmark)

Presentation 2: Dissociative Ionisation Pathways for the Radiosensitiser Mentrionidazole

Daniel Bou Debes (Open University, United Kingdom)

Presentation 3: Ice Mantle Formation in the Interstellar Medium: The Deposition Rate Problem

Matthew D. Dickers (University of Kent, United Kingdom)

Presentation 4: Electron Momentum Spectroscopy of Propylene Oxide

David Matalon (Open University, United Kingdom)

Presentation 5: Electron-Induced Ionisation and Absolute Dissociative Electron Attachment Cross-Section Study of Trans-1,3,3,3-Tetrafluoropropene (HFO1234ze)

Anirban Paul (J. Heyrovský Institute of Physical Chemistry, Czechia)

Presentation 6: Sulphur Implantation in Astrochemical Conditions: Implications for the Jovian System

Ragav Ramachandran (Physical Research Laboratory, India)

Presentation 7: Metal Deposition at Room Temperature: Theoretical Investigation of Precursors for Photoassisted Chemical Vapour Deposition

Cauê Souza (University of Kent, United Kingdom)

Wednesday, 16th October 2024

Conference Day Two (MultiChem Sessions)

Session 4: Electron Interactions with Molecules

Chair: Nigel J. Mason (University of Kent, United Kingdom)

- 09.00 Electron-Induced Processes in Gas and Liquid Phase Molecules
Pamir Nag (J. Heyrovský Institute of Physical Chemistry, Czechia)
- 09.30 Electron and Ion Induced Reactions with Thiophenes Studied by MS, IMS-MS, and DFT
Peter Papp (Comenius University Bratislava, Slovakia)
- 10.00 Electron-Induced Decomposition of Nucleobase Derivatives by Dissociative Electron Attachment Processes
Janina Kopyra (University of Siedlce, Poland)
- 10.30 Electron Collision-Induced Reactions in Isolated and Clustered Interstellar Molecules
Sam Eden (Open University, United Kingdom)
- 11.00 **Coffee Break**
- 11.30 Emission Spectroscopy of Electron-Molecule Collisions
Juraj Országh (Comenius University Bratislava, Slovakia)
- 12.00 Electron-Induced Fragmentation of Biologically Relevant Molecules in the Gas Phase
Stephan Denifl (University of Innsbruck, Austria)
- 12.30 Electron-Molecule Collisions in the Gas Phase
Jelena Maljković (Institute of Physics Belgrade, Serbia)
- 13.00 Experimental and Theoretical Momentum Distributions of Molecules with Astrochemical Relevance
Kate Nixon (Open University, United Kingdom)
- 13.30 **Lunch Break**

Session 5: Radiation Science with Applications to Biology and Health Sciences

Chair: Pamir Nag (J. Heyrovský Institute of Physical Chemistry, Czechia)

- 14.30 Radiation Damage to DNA Nanostructures: From Fundamentals to Applications
Jaroslav Kočišek (J. Heyrovský Institute of Physical Chemistry, Czechia)

- 15.00 Importance of Radiation-Induced Foci (IRIF) in Radiation Research and Health Science
Martin Falk (Czech Academy of Sciences, Czechia)
- 15.30 TBC
Julian Bonello (University of Malta, Malta)
- 16.00 Synthesis and Comprehensive Characterisation of TiO₂ Nanoparticles Doped with Cu and Rare-Earth Elements
Dmitrijs Bočarovs (University of Latvia, Latvia)

Thursday, 17th October 2024

Conference Day Three (COPCA Sessions)

Session 6: Materials Science: Nanosystems, Radiation Research, and Applications

Chair: Maria Alfredsson (University of Kent, United Kingdom)

- 09.30 Manipulating Metal Atoms in Clusters and Nanoalloys to Control Catalysis
Richard Palmer (University of Swansea, United Kingdom)
- 10.00 Radiation Damage and Thermal Annealing Kinetics of Radiation Defects in CVD Diamond Irradiated by Xe Ions
Anatoli I. Popov (University of Latvia, Latvia)
- 10.30 Investigation of Radiation Defects by Thermal Annealing of BaF₂ and CaF₂ Crystals Irradiated with Fast Xenon Ions
Alma Dauletbekova (LN Gulyimov Eurasian National University, Kazakhstan)
- 11.00 **Coffee Break**
- 11.30 Perspectives on Electrochemical Chemosensing
Benji Fenech Salerno (Imperial College London, United Kingdom)
- 12.00 Effect of Irradiation with Swift Heavy Ions on Luminescence of CsI:Tl Crystals
Abdirash Akilbekov (LN Gulyimov Eurasian National University, Kazakhstan)
- 12.30 Analysis of Self-Trapped Hole Mobility in Alkali Halides, Alkaline-Earth Halides and Other Binary and Complex Metal Halides
Marina Konuhova (University of Latvia, Latvia)
- 13.00 **Coffee Break**

14.30 **Excursion to the Mnajdra and Haġar Qim Megalithic Temples**

19.30: **Conference Dinner at the Trattoria AD1530 in Mdina**

Friday, 18th October 2024

Conference Day Four (COPCA Sessions)

Session 7: Space Chemistry I: Radiation-Induced Chemistry and Physics

Chair: Duncan V. Mifsud (HUN-REN Institute for Nuclear Research, Hungary)

09.30 Photodissociation of Molecular Ions Relevant for Astrochemistry and Laboratory Investigation

Sanja Tosić (Institute of Physics, Belgrade)

10.00 Some Experimental Insights into the Microphysics of Ice Processing by Cosmic Rays

Alexei V. Ivlev (Max Planck Institute for Extraterrestrial Physics)

10.30 Ion Processing of Astrophysically Relevant Molecular Systems

Alicja Domaracka (CIMAP-CNRS, France)

11.00 **Coffee Break**

11.30 Ongoing Investigation of Ice Analogues of the Solar System Icy Moons Using Laboratory Facilities

Zuzana Kaňuchová (Slovak Academy of Sciences, Slovakia)

12.00 Radiation Processing of Interstellar Ice Analogues

Sergio Ioppolo (University of Aarhus, Denmark)

12.30 Ion Impact Studies with Astrochemical Relevance

Béla Sulik (HUN-REN Institute for Nuclear Research, Hungary)

13.00 **Coffee Break**

Session 8: Space Chemistry II: Complex Organic Molecules and the Origins of Life

Chair: Sergio Ioppolo (University of Aarhus, Denmark)

14.00 Laboratory Studies on the Radiation-Driven Chemistry in Ices in Space

Duncan V. Mifsud (HUN-REN Institute for Nuclear Research, Hungary)

14.30 Low (10 K) and High Temperature (10⁴ K) Astrochemistry

Bhalamurugan Sivaraman (Physical Research Laboratory, India)

- 15.00 Reactive Collisions of Small Aromatic Compounds with Atoms / Radicals by the
 Crossed Molecular Beam Technique
Gianmarco Vanuzzo (University of Perugia, Italy)
- 15.30 A Systematic IR and VUV Spectroscopic Investigation of Ion, Electron, and Thermally
 Processed Ethanolamine Ice
Jin Zhang (Queen Mary University of London, United Kingdom)
- 16.00 Fragmentation of Complex Organic Molecules: Exploring Pathways to Prebiotic
 Precursors
Heidy M. Qutián-Lara (Max Plank Institute for Extraterrestrial Physics, Germany)
- 16.30 **Conference Closing**

Progress in Multiscale Computational Modelling of Meso-Bio-Nano Systems Exposed to Radiation

Andrey V. Solov'yov

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This talk will present the roadmap paper written by a group of members of the COST Action MultiChem [1]. It will review the new highly interdisciplinary research field studying the behaviour of condensed matter systems exposed to radiation and will highlight several relevant examples of recent advances in the field. Condensed matter systems exposed to radiation may have very different natures, being inorganic, organic or biological, finite or infinite, be composed of many different molecular species or materials, existing in different phases (solid, liquid, gaseous or plasma) and operating under different thermodynamic conditions. The essential and novel element of this research is that, despite the vast diversity of such systems, many of the key phenomena related to the behaviour of irradiated systems (such as radiation-induced damage, mechanisms of damage repair and control, radiation protection, etc.) are very similar and can be understood based on the same fundamental theoretical principles and computational approaches [1]. One of the essential features of the aforementioned phenomena concerns their multiscale nature as the manifestation of the radiation-induced effects occurring at different spatial and temporal scales ranging from the atomic to the macroscopic [2,3]. The multiscale nature of the effects and similarity of their manifestation in systems of different origins necessarily brings together different disciplines, such as physics, chemistry, biology, materials and nano-science, and biomedical research, demonstrating numerous

interlinks and commonalities between them [2,3]. This research field is highly relevant to many novel and emerging technologies [4,5] and medical applications [6]. Several computational multiscale case studies reported in [1] will be presented.

References

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Applications of Multiscale Modelling in Astrochemistry and Nanofabrication

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Synopsis. This work explores the applications of multiscale modelling techniques in astrochemistry and nanofabrication to understand complex chemical phenomena across different scales. In astrochemistry, computational methods are employed to investigate the structural and spectroscopic properties of interstellar fullerenes and their hydrogenated derivatives, providing insights into their potential roles as carriers of diffuse interstellar bands. Additionally, the fragmentation pathways of saturated organic molecules in the interstellar medium are studied to elucidate the formation of unsaturated species with extended π -bond networks under high-energy conditions. In nanofabrication, quantum mechanics and molecular dynamics simulations are applied to model photoassisted chemical vapour deposition (PACVD) processes. This includes developing substrate models, investigating the photochemistry of precursors, and simulating the deposition process. By integrating multiscale modelling approaches, the work aims to enhance the understanding of complex chemical processes, thereby contributing to advancements in both astrochemical research and nanofabrication technologies.

Multiscale modelling serves as a crucial bridge between the microscopic interactions of atoms and molecules and the macroscopic phenomena observed in complex chemical systems. By integrating computational techniques across different scales—from quantum mechanics, which describe electronic interactions, to molecular dynamics, which simulate the behaviour of larger assemblies over extended time-scales—a comprehensive understanding of chemical processes can be achieved, even when direct experimental observation is challenging.

In this talk, the potential of multiscale modelling will be highlighted through its application in two distinct yet somehow interconnected fields: astrochemistry and nanofabrication.

Part I: Applications in Astrochemistry

The discovery of fullerenes such as C_{60} , C_{60}^+ , and C_{70} in the interstellar medium (ISM) has spurred significant interest in

their formation, stability, and role in cosmic environments.¹ Using density functional theory (DFT) and automated global minimum search algorithms, we investigated the structural and spectroscopic properties of gas-phase $C_{60}H_n^{q+}$ hydrogenated fullerenes, or fulleranes ($n = 0-4$ and $q = 0,1$). Our studies revealed novel global minimum structures for these species, highlighting how hydrogenation alters their ionisation potentials and proton affinities. These findings have important implications for the detection and role of these molecules in the ISM.²

One key challenge in astrochemistry is identifying molecules that contribute to diffuse interstellar bands (DIBs). We found that traditional mid-infrared and UV-Vis spectroscopy may not reliably detect neutral fullerenes. However, we identified distinctive electronic transitions in the near-infrared range, which could serve as unique markers for cationic fullerenes.² This opens up new possibilities for future astronomical

observations to detect these molecules in space.

Further work by us³ explored the fragmentation pathways of saturated organic molecules such as ethanolamine, propanol, butanenitrile, and glycolamide under high-energy conditions in the ISM. Using electron-impact ionisation data and Born–Oppenheimer molecular dynamics simulations, we demonstrated that energetic processes—such as cosmic rays and shock-induced heating—can transform these saturated molecules into unsaturated species with extended π -bond networks. This provides valuable insights into the chemical evolution of organic molecules in dense molecular clouds like Sagittarius B2, shedding light on how complex organic species form in space.

Part II: Applications in Nanofabrication

In nanofabrication, multiscale modelling has been employed by us to simulate photoassisted chemical vapour deposition (PACVD) processes,⁴ which are used to deposit thin metal films at near-room temperature, essential for working with thermosensitive substrates.

Detailed molecular mechanics models of alkanethiol self-assembled monolayers (SAMs) on gold surfaces were developed by us, as these SAMs serve as substrates in PACVD. Through simulations using the MBN Explorer software,⁵ the ligand tilt angles relative to the surface normal—an essential factor influencing the quality of the deposited films—were accurately modelled. We showed that non-bonded force field parameters, such as Lennard-Jones potentials and partial charges, play a significant role in determining these tilt angles. These findings provide guidance for more accurate SAM models in future nanofabrication studies.

Additionally, the photodissociation properties of polyhapto ruthenium-based precursors, used in PACVD, were explored by us using time-dependent DFT calculations. By mapping excited-state potential energy surfaces and identifying key dissociation channels, molecular-level insights into the PACVD process were obtained. This understanding is crucial for optimising precursor molecules and deposition conditions, enhancing the precision and efficiency of nanofabrication techniques.

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Understanding the Spin States in Coordination Complexes

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Synopsis. Understanding the spin-states in coordination complexes is crucial for predicting their chemical (re)activity, magnetic properties, and potential applications. This research focuses on the theoretical and computational analysis of spin-states in transition metal complexes based on density functional theory. The study examines ligand field strength, metal-ligand covalency, and electronic correlation. Case studies include manganocene, Fe(III) and Mn(II) complexes with bis-tridentate Schiff base ligand, and spin-crossover pentagonal bipyramidal complexes. The results highlight the interplay between these factors and their impact on the observed spin-states, providing insights into the design of novel coordination complexes with tailored properties. This work aims to advance the understanding of spin-state phenomena, paving the way for innovations in catalysis and materials science.

The electronic structure of a molecule determines all its properties. In the case of transition metal (TM) complexes, the electronic structure depends on the number, geometry, and character of metal-ligand bonds [1]. A particular challenge in understanding the electronic structure of TM complexes is related to the partially filled metal *d* orbitals. This leads to different, energetically accessible ways to distribute the same number of *d*-electrons. For example, in a hexacoordinated environment, the different spin ground state is observed with TM ions having four to seven *d*-electrons: with a maximum number of unpaired electrons, leading to the high-spin state, or with none or minimal numbers of unpaired electrons – giving the low-spin state. Any intermediate arrangement is called the intermediate-spin state. The spin state of a coordination complex plays a crucial role in determining its chemical reactivity, magnetic properties, and potential applications in catalysis and materials science [2].

This talk will delve into the theoretical and computational approaches used to understand and predict the spin-states of

coordination complexes, focusing on density functional theory (DFT) calculations. We will explore the factors influencing spin-state energetics, including ligand field strength, metal-ligand covalency, and the role of electronic correlation. Four case studies will illustrate the interplay between these factors and their impact on the observed spin-states. Additionally, we will discuss the challenges and limitations of current computational methods in accurately predicting spin-states.

Case studies

1. Manganocene. Manganocene is an organometallic compound with unique characteristics that set it apart from other known sandwich compounds. Its properties are explained by the interplay of the degenerate ground state and close-lying electronic and spin states [3].

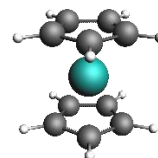


Figure 1. Structure of manganocene

2. Fe(III) and Mn(II) complexes with bis-tridentate thiosemicarbazone ligand.

Mn(II) and Fe(III) complexes with a condensation product of thiosemicarbazide and 2-acetylthiazole have the same d^5 electronic configuration but show different coordination geometries, spin-states, and biological activities. High-spin Mn(II) complex has trigonal-prismatic geometry with ionic metal-ligand bonding, while low-spin Fe(III) is octahedral with strong metal-ligand and covalency [4].

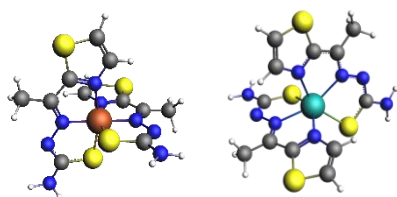


Figure 2. Structure of low-spin Fe(III) (left) and high-spin Mn(II) (right) complexes with thiosemicarbazone ligand

3. Intermediate-Spin Iron(III) Complexes.

A square pyramidal Fe(III) complexes with N_2S_2 tetradentate ligand and halogenido ligand show unusual intermediate-spin ground state as a consequence of strong and covalent bonding in the equatorial plane and weak bonding between metal and axial ligand [5].

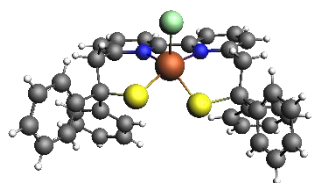


Figure 3. Structure of intermediate-spin Fe(III) complexes

4. Spin-states in seven-coordinate complexes.

Spin-crossover Fe(II) complex with N_3O_2 pentadentate macrocyclic ligand and two cyano axial ligands show unusual features when going from the low-spin to the high-spin state. This spin-state change induces changes in the coordination

environment from hexacoordinate to heptacoordinated [6].

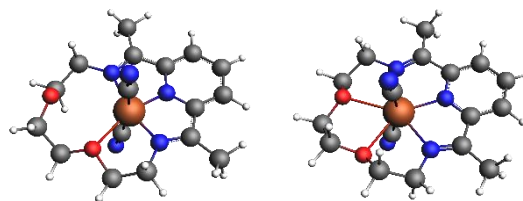


Figure 3. Structure of hexacoordinated low-spin Fe(II) (left) and heptacoordinated high-spin Fe(II) complexes.

Conclusions

By providing a comprehensive understanding of spin-state phenomena, this presentation aims to contribute to the design of novel coordination complexes with tailored properties for specific applications. This knowledge will pave the way for advancements in catalysis, materials science, and beyond.

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Modelling Collision Processes in Complex Molecular Systems Using VIKING

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Collisions within complex molecular systems have emerged as a critical field of scientific research, offering profound insights into diverse applications such as cancer therapy [1], tissue protection in extreme environments (e.g., space) [2], and spectroscopy techniques like point projection microscopy (PPM) [3]. Achieving an accurate theoretical description of these processes requires a comprehensive approach that spans multiple scales. This encompasses capturing the interplay between quantum mechanical effects at the microscale and the subsequent influence on molecular structures at larger time and length scales.

At the microscopic level, accurately modelling the interaction between colliding particles presents non-trivial challenges due to the importance of quantum mechanical effects. To address these challenges, real-time dependent density functional theory (RTDDFT) has proven to be an effective tool [1]. However, the complex nature of RTDDFT limits its accessibility to select scientific groups.

To overcome these limitations and promote wider usage, we introduce a new task into VIKING [4], a web-based scientific framework focused on addressing multiscale problems (Fig. 1). VIKING [4] combines different theories and programme packages, providing an easy-to-use yet accurate implementation of various methods across different scales. In this work, we present the newly integrated collision task

within VIKING, specifically designed to describe the interactions between arbitrary molecular systems and different types of colliding particles, such as ions, electrons, and photons. Moreover, the collision task in VIKING offers a portfolio of adjustable parameters, including geometry optimisations, automatic rotations of impact angles, and velocity distributions, all of which are evaluated automatically. By offering this flexibility, the collision task in VIKING enables researchers to tailor their simulations to specific scenarios and explore the impact of various factors on collision outcomes.

Overall, the integration of the collision task within VIKING provides a user-friendly platform for researchers from diverse scientific backgrounds to investigate the dynamics of particle collisions within molecular systems, yielding valuable insights into a wide range of applications.

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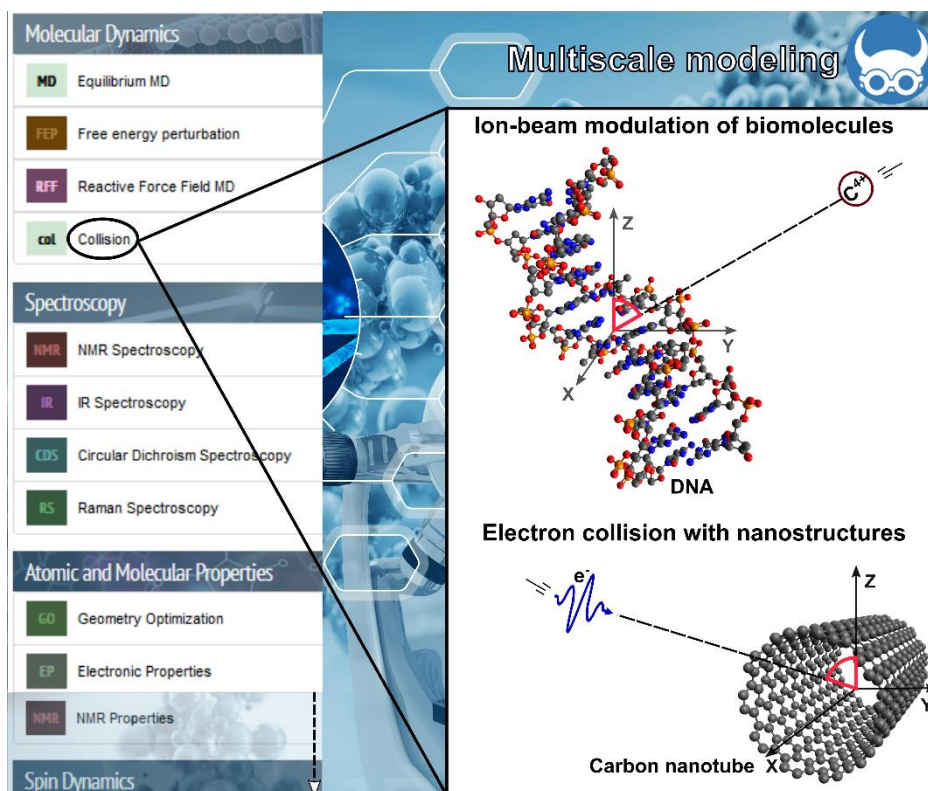


Figure 1. VIKING facilitates a comprehensive multiscale approach for various systems by offering multiple interconnected tasks (left side). A notable addition to VIKING is the collision task, which enables the investigation of diverse collision scenarios, spanning from ion-beam collisions to interactions between fast electrons and nanostructures. Moreover, VIKING boasts a user-friendly web-based GUI, which facilitates efficient parameter screening, including the adjustment of collision angles (highlighted in red).

Radiation-Induced Phenomena in Molecular and Atomic Cluster Systems Studied with MBN Explorer and MBN Studio

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Synopsis. This talk will present several recent examples of the successful application of the MBN Explorer software package for atomistic simulations of radiation-driven processes in molecular and condensed matter systems. Particular examples will include simulations of the radiation-induced fragmentation of organometallic precursor molecules and structural transformations in deposited metal clusters induced by the focused electron beam of a scanning transmission electron microscope.

Irradiation-Driven Molecular Dynamics (IDMD) [1] is the advanced computational method implemented in the MBN Explorer software package [2], which enables atomistic simulations of irradiation-driven transformations in various Meso-Bio-Nano (MBN) systems. Within the IDMD framework, different quantum processes occurring in an irradiated system (e.g., covalent bond breakage induced by ionization or electron attachment) are treated as random, fast, and local transformations, which are incorporated into the classical MD framework in a stochastic manner, with probabilities elaborated on the basis of quantum mechanics [1]. Major transformations of irradiated molecular systems (such as changes in molecular topology, redistribution of atomic partial charges, or changes in interatomic interactions) are simulated using the reactive CHARMM (rCHARMM) force field [3] implemented in MBN Explorer.

IDMD relies on several input parameters, such as bond dissociation energies, molecular fragmentation cross sections, the amount of energy transferred to the system upon irradiation, the energy relaxation rate, and the spatial region in which the energy is relaxed. These characteristics can be obtained by accurate quantum mechanical calculations, e.g. by means of density

functional theory (DFT) and time-dependent DFT. Alternatively, the required parameters can be obtained from experimental data or by analytical models and methods [4-6].

Due to the countable number of physical parameters, together with a much larger number of different output properties available for simulation and analysis, the IDMD method [1] offers unique possibilities for modelling irradiation-driven modifications and chemistry of complex molecular systems beyond the capabilities of either pure quantum or pure classical MD [7].

The talk will present several case studies illustrating the use of IDMD and its validation by comparison with experiments. Particular examples include simulations of the radiation-induced fragmentation of organometallic precursor molecules [8, 9].

Finally, the presentation will present the results of the recent study [10] devoted to the analysis of structural transformations in deposited metal clusters induced by the focused electron beam of a scanning transmission electron microscope. In this context, the application of the relativistic MD approach [11], another unique and powerful methodology implemented in MBN Explorer, to simulate the collisions of

energetic primary electrons with cluster atoms, will be illustrated.

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Atmospheric Pressure Low-Temperature Plasma for Application in Agriculture and Food Processing

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Synopsis. Application of cold atmospheric pressure plasma is promising technology in the field of agriculture and food industry for decontamination, improvement of germination, growth and physiological parameters, reduction of chemicals, increase of food safety and extending shelf-life of food products. In addition, current research also points to the ability to initialize adaptation and repair mechanisms in biological samples, e.g plant seeds or microorganisms, which represents a huge potential in solving problems that agriculture and food industry is currently facing – increase of population, climate changes, environmental pollution, crops diseases, and decrease of food quality.

Plasma technologies is in present a prospective alternative to standard wet chemical processes in industry with significantly less chemicals and time-consuming approach. Within the development of plasma sources generating low-temperature plasma at atmospheric pressure, so called *Cold atmospheric pressure plasma (CAPP)*, the application of plasma found their wide use in treatment of biological material in the field of medicine, agriculture and food processing^{1,2}.

In the food industry, CAPP is utilized for the decontamination of food products, ensuring the microbial safety of products without altering their sensory qualities or nutritional value and for modification of surfaces in food packaging. This technique is particularly attractive due to its environmentally friendly nature, as it reduces the reliance on chemical preservatives and high-temperature processing³.

In agriculture, plasma application primarily focuses on seed treatment, where plasma promotes faster germination and enhances the seeds' ability to withstand

environmental stresses. Additionally, it contributes to the elimination of pathogens on seed surfaces, thereby reducing the need for chemical pesticides and seed dressing^{4,5}.

Research shows that plasma also plays a significant role in improving plant health by activating defense mechanisms, increase the resistance to pathogens and enhancing nutrient absorption⁶. Studies focused on interaction of plasma with biological materials such as cells, microorganisms, and seeds have demonstrated that cold plasma can stimulate protective mechanisms in these organisms, for example, by increasing the production of antioxidant enzymes or enhancing DNA repair mechanisms. This phenomenon is often referred to as the "plasma-induced adaptive response" and it contributes to increasing the resilience of organisms against stress factors such as UV radiation, drought, environmental pollution or pathogens⁷.

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Exploring Electrical Breakdown in Ultra-Low Global Warming Potential Gases for Insulation in Medium and High-Voltage Technology

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Synopsis. In response to growing environmental concerns associated with SF₆ gas for insulation in medium and high-voltage technologies, a new class of gases eco-friendly gases has emerged as a potential alternative. Our work explores the breakdown properties of these fluorocarbon gases with low Global Warming Potential and Low Ozone Depletion potential. By sustaining discharge under swarm conditions at low currents and pressures, we can determine breakdown voltages, ionisation coefficients, and secondary electron yields. Measured parameters may be used directly in plasma modelling and to extend normalising sets of cross-sections to high mean energies.

Recently developed hydrofluoroolefins (HFOs), perfluoroketones (PFKs) and perfluoronitriles (PFNs) with a low impact on the climate are nowadays in the focus of the community, having in mind the lack of relevant data required for application to environmentally benign power equipment [1]. Our motivation extends to applying these gases in resistive plate chamber particle detectors, where a mixture of greenhouse gases (C₂H₂F₄, SF₆ and i-C₄H₁₀) is currently used [2].

Our measurements are done in a centimetre-sized plan-parallel electrode system, under swarm conditions at low currents (~ 1 μA) and low pressures (~0.1 – 1 Torr). Results include optical emission spectra, spatially and spectrally resolved distributions of discharge emission, effective ionisation coefficients, secondary electron yields and Paschen curves. The breakdown and voltage-current measurements, together with the results for effective ionisation coefficients, allow the development of complete sets of cross-sections and other

discharge parameters in the mean energy region relevant to numerous applications.

In Figure 1, we present breakdown results for 1,1,1,2-Tetrafluoroethane (R134a, C₂H₂F₄) and 2,3,3,3-Tetrafluoropropene (HFO-1234yf, C₃H₂F₄), in comparison with selected conventionally used fluorocarbons.

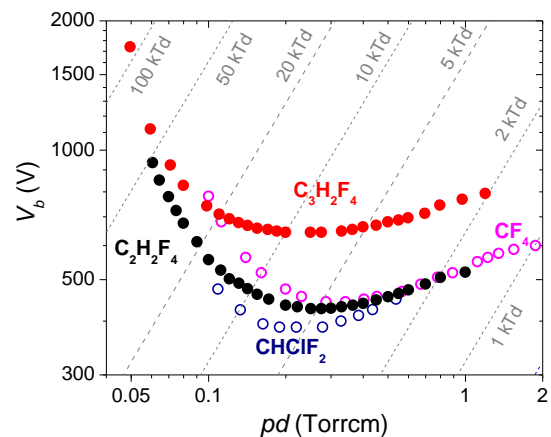


Figure 1 Paschen curves of R134a and HFO-1234yf, compared to CF₄ and CHClF₂ (R-22).

From spatially and spectrally resolved emission profiles, we can determine effective ionisation coefficients [4] at high values of density-normalized electric fields (E/N) (Figure 2).

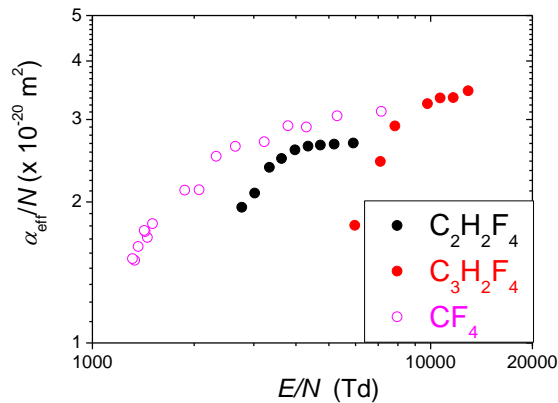


Figure 2. Effective ionisation coefficients.

With the highest breakdown voltages and ionisation coefficients pushed towards the highest E/N -s, HFO-1234yf shows the best potential for insulation. It is not a satisfactory SF_6 alternative but represents a step toward understanding elementary processes in these complex new gases.

Acknowledgements

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Computational Studies of Redox-Active Transition Metal Compounds

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Synopsis. We discuss how electronic structure calculations can be employed to provide atomic level information on structures and properties of compounds containing redox-active transition metal ions. We examine recent applications in heterogeneous catalysis and energy storage to exemplify surface and bulk processes. The complementarity of computational and experimental information is discussed.

Electronic structure calculations play an important role in the study of functional materials, where they provide atomic level information complementary to experiment.

In this presentation we examine two recent application areas, both exploiting the redox activity of transition metal ions in an inorganic matrix. The first example is oxidation catalysis in metal-doped and metal exchanged zeolites. Transition metal ions in AlPO frameworks are active oxidation catalysts, able to exploit molecular oxygen as reactant for the selective oxidation of the terminal C in hydrocarbons [1]; Cu-exchanged zeolites are instead employed as de-NO_x catalysts in the treatment of diesel exhaust flues [2]. In both cases, the challenge for the design of improved catalytic materials is to identify the exact mechanistic pathway. While challenging for experimental probes, this detail is now available from computational studies.

The second application area presented is that of energy storage materials. We exemplify this work with the study of cathode materials in Li-ion [3] and post-Li ion batteries [4]. These must be able to accommodate the reversible intercalation of cations in a crystalline host and allow facile movement of the intercalated species. Despite the different applications, both materials

examined exploit the redox activity of transition metal ions and require the estimation of barriers for atomic level processes.

Other than the practical applications, electronic structure studies of redox-active transition metals are a theoretical challenge because Density Functional Theory (DFT), the method of choice for electronic structure studies of crystalline solids, has known limitations in describing localised electrons like those in the 3d states of the active metal ions. We show how the choice of functional in DFT is critical, with hybrid-exchange functional being required for accurate results.

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Advancing the Performance of Li-Ion Batteries Using X-rays

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Synopsis. Energy storage is important in many applications from transport, portable electronics to microelectronics and with the increased demand we need to find low cost materials that are environmental friendly, non-toxic, and sustainable. Iron-based polyanion compounds, full-fill many of these expectations and LiFePO₄ (LFP) is one of the commercial material widely used. As cathode material in Li-ion batteries, LFP demonstrate good specific capacity (170 mAhg⁻¹), but low operational voltage and conductivity driving the demand for further development. In this work we will present how synchrotron radiation can be employed to identify how doping and modifications in the electrode composite improve the electrochemical performance of LFP while working towards a greener manufacturing process.

Despite the commercial benefits associated with lithium iron phosphate (LFP), it is well-known to suffer from poor electronic and ionic conductivity as well as low effective voltage, issues that been addressed by carbon-coating, nanosizing, and cation doping. The interest of materials with polyanionic oxide groups (XO₄^{y-}) for energy storage has been increasing due to the ability of the covalent polyanion groups to lower the energy of the active redox couple to a more functional range and to increase the working voltage through the stabilisation of the redox couple through the X-O covalency.

Minimal quantities of dopant can distort the crystal structure of LFP resulting in higher Li-ion diffusion. Dopants, such as Mo⁴⁺, Al³⁺, V³⁺, Zr⁴⁺, and W⁶⁺ have been reported to improve the ionic conductivity of LFP by around 7 orders of magnitude ($>10^{-2}$ S cm⁻¹ vs 10^{-9} - 10^{-8} S cm⁻¹).¹ Rare-earths, such as Ho and Dy has been less studied in the literature, but due to their ionic radii they can be expected to introduce further distortion improving ionic conductivity in the material. Instead mixed-cation LiFe_{1-x}Mn_xPO₄ (LFMP) offers a potential

solution, toward increased operational voltage. The ongoing debate surrounds the redox activity of manganese (Mn) in this compound.

XAS has been used as an analytical technique for LFP and, its doped analogues. This study aims to follow the Fe, P, and dopant (V, Ho and Mn) K-edges in order to study the effects of the dopant cation on the material, and to further understand the activity of the phosphate polyanion by quantifying the dipole inductive effect as a battery is cycled. Through XAS, electrochemical analyses, and linear combination fittings we are able to analyse and comprehend the chemistries and behaviours of these materials and understand the use and impact of dopant cations as a method for the improvement of LFP cathodes.

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Electron Induced Processes in Gas- and Liquid-Phase Molecules

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Synopsis. The talk will be divided into two parts. In the first part, I will discuss low-energy electron collision processes with gas-phase molecules. We have utilized a VMI spectrometer to investigate dissociative electron attachment (DEA) to astrophysically significant isoelectronic molecules NCCN and HCCCN. Additionally, I will present ongoing results of DEA to CH₃I. In the second part, I will introduce our new experimental setup designed to study electron-induced reactions with liquid and solvated-phase molecules, along with updates on current results.

Low-energy electron molecule scattering often leads to the formation of anionic states via resonant electron capture, which may result in dissociative electron attachment (DEA). In Prague, we possess a unique DEA-VMI (velocity map imaging) spectrometer combined with a trochoidal electron monochromator [1]. Recently, we measured the VMI of CN⁻ produced due to DEA to two isoelectronic, astrophysically important molecules – NCCN and HCCCN. Despite their similarity, these molecules exhibited contrasting dynamics in anion formation due to low-energy electron attachment [2].

The VMI spectrometer can produce an electron beam as low as 10 meV, enabling us to conduct DEA-VMI experiments around zero-eV resonances. Recently, we have measured the VMI of the I⁻ anion produced due to DEA to the CH₃I molecule around zero eV. Previously, the effect of vibrational Feshbach resonances was observed in the DEA cross section of I⁻/CH₃I [3], but no report of angular distribution of VMI data has been available until now due to the lack of suitable experimental apparatus. The VMI spectra of I⁻/CH₃I measured at 0.01 eV incident electron energy are shown in Figure 1(a).

In Prague, we have also recently developed a new experimental setup to study electron beam-induced processes in liquid- and solvated-phase molecules. One motivation for this work is to understand the radiation-induced damage to living cells and biologically important molecules in their natural environment – i.e., in aqueous solvated form. In the second part of the talk, I will discuss recent results.

We used the setup to study electron-beam-induced reactivity in water-solvated TRIS (2-Amino-2-(hydroxymethyl) propane-1,3-diol) molecule mediated via secondary OH radicals produced due to primary electron irradiation. We employed UV-Vis spectroscopy to understand the effect [4].

We also investigated different molecules like disodium terephthalate and coumarin carboxylic acid with the aim of developing accurate in-situ chemical dosimeters. Fluorescence spectrometry was used to study the effect of secondary OH radical-induced processes. These works are currently in progress. In the talk, I will provide a progress report. The sample fluorescence spectra of

a 5mM aqueous solution of disodium terephthalate, after 600 eV energy electron beam irradiation, are shown in Figure 1(b).

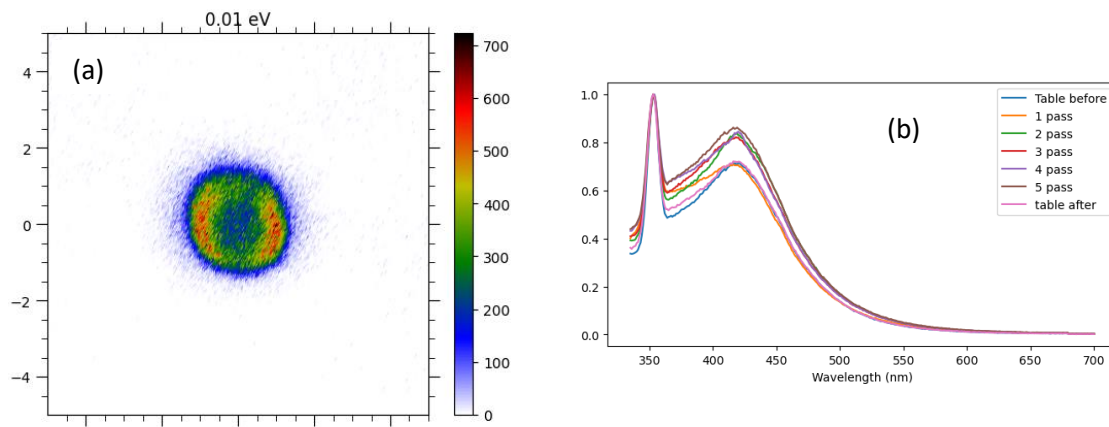


Fig. 1 (a) The time sliced velocity map image of I^- ions produced due to DEA to CH_3I molecule at 10 meV incident electron energy is shown here. (b) The fluorescence spectra of aqueous solution of disodium terephthalate after irradiation with 600 eV electron beam is shown here. The fluorescence spectra are measured at 315 nm excitation wavelength.

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Electron and Ion Induced Reactions with Thiophenes Studied by MS, IMS-MS and DFT

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Synopsis. Sulphur containing hydrocarbons are being studied experimentally and theoretically. Thiophene (T), methyl (2MT) and dimethyl (2,5DMT) thiophene together with benzothiophene (BT) and dimethyl benzothiophene (2MBT) have been studied. Low-energy electron interactions studied by mass spectrometry (MS) and ion-molecular processes studied by ion mobility spectrometry (IMS-MS) have been interpreted with DFT calculations.

In this work, electron and ion induced processes are of main interest, represented by dissociative ionization, dissociative electron attachment, as well as charge transfer reactions. Sulphur containing compounds thiophene, 2-methyl thiophene, 2,5-dimethyl thiophene, benzothiophene and 2-methyl benzothiophene are being discussed. For petronel industry, sulphur containing compounds are considered as contaminants, in crude oil are among the most abundant constituents, in some cases as high as 10% [1]. However, going further from earth conditions, sulphur is considered to be the tenth most abundant element in the universe and is known to play a significant role in biological systems, investigation of sulphur containing astrochemical molecules is therefore of high interest [2]. Either sulphur containing hydrocarbons are of high interest, among all possible chemicals five- or six-member rings containing sulphur atom as well.

Electron induced MS together with Atmospheric Pressure Chemical Ionization used in IMS-MS at Comenius University in Bratislava [3,4,5] is being used to study the above-mentioned processes. Quantum chemistry is used to model the thermochemical properties, ionization energies,

electron affinities, bond energies in ions, proton affinities and reactions leading to formation of ions and charged clusters of the studied analytes.

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Electron-Induced Decomposition of Nucleobase Derivatives by Dissociative Electron Attachment Processes

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Synopsis. In this contribution, we report on the interaction of low energy (< 12 eV) electrons with thio-derivatives of pyrimidines, the compounds that apart from the sulphur atom contain an additional (N) heteroatom within the six-membered ring or an electron-affinic side group -COOH. In addition to the formation of molecular anions, we observe the production of several different negatively charged fragments arising from low-lying resonances. These data will be discussed in the context of previously reported DEA results for native pyrimidines and thio-nucleosides.

Reactions triggered by electron capture into molecules, including those that result in molecular dissociation, play a crucial role in many essential areas, such as (nano)technology, chemical engineering, atmosphere, astrochemistry, radiation physics and chemistry, and radiation therapy [1].

In recent decades, there has been considerable interest in studying the interactions of low-energy electrons with biologically important molecules. Among these, many experimental and theoretical studies have been devoted to complex biostructures like DNA and its subunits [2,3] in order to discover the molecular mechanism by which low energy electrons (LEEs) damage macromolecules. Recently, much research has been devoted to compounds that may act as potential radiosensitisers in cancer therapy. Such compounds can be represented, for example, by modified bases, nucleosides, and nucleotides by introducing halogen atoms into the molecular structure. Some of these compounds show supra-additive cytotoxic effect when combined with radiation, meaning that the reduction of tumour tissue is more effective in combination than the sum of the individual effects of chemotherapy and radiotherapy.

In the present contribution I shall present a gas phase dissociative electron attachment study of biologically relevant compounds consisting of six-membered rings with two or more heteroatoms and fused carbocyclic derivatives, namely 5-carboxy-2-thiouracil, 6-azauracil, and 6-aza-2-thiothymine

conducted in a crossed beam experiment under single collision conditions. Such chemical compounds are often used as biological modifiers capable of altering the response to radiation. Nowadays, radiation-induced responses are increasingly used to modify radiotherapy based on advances in radiobiology. Therefore, it is necessary to determine the behaviour of these halo-substituted subunits under reducing conditions. In particular, focus of the talk will be on describing the formation of negative ion transitions and comparing the fragmentation patterns of a series of (aza)pyrimidines.

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Electron Collision-Induced Reactions in Isolated and Clustered Interstellar Molecules

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Synopsis. Metastable dissociative ionization experiments and DFT calculations reveal new insights into the fragmentation pathways of benzonitrile that are unavailable from conventional mass spectrometry. Further experiments and calculations explore radiation-induced intermolecular reactions in benzonitrile cluster ions, including new routes to produce interstellar polycyclic aromatic hydrocarbon (PAH) ions.

Since benzonitrile's discovery in the interstellar medium (ISM) in 2018 [1], several studies have explored the strongest unimolecular dissociations of its radical cation [2, 3]. However, no investigation has been conducted to date on its sequential dissociation and this can be an important source of reactive products. Metastable dissociative ionization experiments enable a dissociation's precursor ion and its product ion to be identified simultaneously [4], and hence can distinguish sequential fragmentation pathways.

This talk will report multi-photon ionization (MPI) and electron ionization (EI) metastable dissociation experiments on gas-phase benzonitrile. They reveal 11 new dissociations, 9 of which involve the dissociation of a fragment ion. We observe CH[•] and C₃H[•] from ionized benzonitrile for the first time, as well new dissociations producing the astrochemically-important reactants HCN / CNH and CN[•]. A further highlight is identifying C₆H₂N⁺ production following H loss from ionized benzonitrile. This enables the presence of C₆H₂N⁺ in the ISM to be inferred for the first time. DFT calculations were performed to elucidate the reactions

responsible for the newly observed dissociations.

Further to the gas-phase studies described above, the talk will report ionization experiments and calculations on benzonitrile clusters. Reactions on dust or ice surfaces are understood to be critically important in interstellar chemistry, and clusters provide model systems to identify condensed-phase intermolecular reactions. We elucidate proton transfer reactions in benzonitrile cluster ions for first time, and we observe a novel dehydrogenated dimer ion product. DFT calculations (originally aimed at understanding dehydrogenated dimer ion production) reveal another reaction pathway that produces a new PAH ion with the same *m/z* value as the benzonitrile dimer ion.

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Emission Spectroscopy of Electron-Molecule Collisions

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Synopsis. Electron-molecule collisions play an important role in various environments from natural phenomena through laboratory to industry. The low-energy collisions produce a wide array of neutral, excited, or charged products. The combination of emission spectroscopy as an analytical method to detect excited products and study excitation reactions and crossed-beams experimental technique provides the possibility to examine the reactions at very well defined conditions. The resulting data can serve as a reference for deeper analysis of radiation emitted by complex sources such as plasmas, discharges, comets, atmospheres of various celestial bodies, stars, etc.

Emission spectroscopy is a tool often used to analyse systems such as electrical discharges, atmospheric processes or various interstellar objects. The emission from these objects is often very complex as many different processes producing emission can be active at once and local conditions can affect the shapes of spectral features. Such a complex spectrum contains many valuable information on its source but can be difficult to analyse. In many of these environments the electron induced processes play an important role. Even in astrophysical conditions it was shown that slow secondary electrons generated by photoionization induce significant portion of radiation emitting particles [1]. Therefore, the laboratory experiments aimed at electron induced fluorescence can provide the reference data, since they work in controlled environment repeatably studying individual compounds. The figure 1 shows the example of the spectral electron energy map of nitrogen emission induced by electron impact. The main output are the reference emission spectra determined at range of electron energies providing the possibility to extract absolute emission cross-section values for all the detected transitions at any energy.

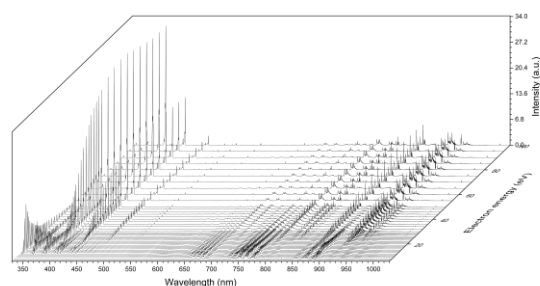


Fig. 1. Spectral electron energy map of nitrogen [2].

Acknowledgments

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Electron-Induced Fragmentation of Biologically Relevant Molecules in the Gas Phase

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Synopsis. In this contribution I will present highlights of our recent electron attachment studies with biologically relevant molecules in the gas phase. Electron attachment represents an important process in different biological systems and thus studies about electron attachment provide fundamental knowledge about the related basic properties of biologically relevant molecules. We used crossed electron-molecule beam experiments for studying anion formation upon low-energy electron attachment. The anionic species was detected by mass spectrometry. Our electron attachment studies with triazole compounds indicate a strongly modified fragmentation behaviour upon addition of a NO₂ group. I will also briefly summarize results for sanazole and RRX-001 compounds, which indicate that the presence of NO₂ group within the molecular frame may be exploited in these systems for radiosensitization as well.

Electron attachment of a free or bound electron to molecules is a fundamental process in nature and may be also exploited for technical or medical applications. In particular, it may be used for generation of radicals, which subsequently lead to a chemical transformation of matter. The negative ion formed by electron attachment may itself be the active species or alternatively, the electron attachment process may lead to dissociation of the molecule, forming reactive fragments in either neutral or charged form. Free electrons are generated in matter during irradiation by energetic radiation. While natural biological tissue may have a limited response towards such irradiation (in particular, when molecular oxygen is missing), various types of molecules have been considered to substantially increase the effects of irradiation. Such molecules, called radiosensitizers, have been for example suggested for hypoxic tumor tissue which is characterized by a lack of oxygen [1]. It is then the question, which molecular design maximises the effect of sensitization. It is well known, that certain nitroimidazolic

compounds mimic the oxygen effect very well. Assuming that electron attachment is a relevant process in activation of nitroimidazoles, the addition of NO₂ groups should considerably improve the molecular properties with respect to anion formation. We recently investigated this hypothesis by studying electron attachment to the potential radiosensitizers RRX-001, sanazole and 3-nitrotriazole [2]. For the latter molecule, comparison with native triazole indicates strong improvement of electron capturing abilities in 3-nitrotriazole. To reveal these effects, we experimentally used an electron monochromator to generate a well-defined electron beam. We coupled it with a quadrupole mass spectrometer to identify the anions formed by electron attachment.

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Electron Molecule Interaction in the Gas Phase

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Synopsis. We have undertaken a collaborative study combining theoretical and experimental approaches to investigate elastic electron scattering from halotahane, sevoflurane, isoflurane and desflurane, considering the environmental impact of these halogenated compounds. In our experimental work, elastic differential cross sections (DCS) were measured at an electron energy range from 50 eV-300 eV. using a crossed-beam apparatus equipped with an electron gun, a capillary gas needle, and a channeltron detection system. Theoretical calculations were performed using the Independent Atom Model with the Screening Corrected Additivity Rule (IAM-SCAR+I), incorporating interference effects.

Considering the growing interest for the environmental impact of anesthetic molecules on both global warming and ozone layer depletion, we have undertaken a collaborative study combining theoretical and experimental approaches to investigate elastic electron scattering from halothane, sevoflurane, isoflurane, and desflurane. These anesthetic gases, commonly excreted unchanged into the atmosphere after use [1], contribute to rising global concentrations of halogenated compounds, which possess high Global Warming Potentials (GWP) and significant Ozone Depletion Potentials (ODP).

Crossed electron-molecular beam apparatus UGRA was used for measuring absolute differential cross sections for elastic electron scattering on anesthetic molecules. The experimental set-up consists of an electron gun (hairpin electron source, up to about 1 μ A incident beam current in the energy range from 50-300 eV) a double cylindrical mirror energy analyzer

(DCMA) and a channel electron multiplier as a detector [2]. The experiment is performed in crossed beam setting. Relative differential cross section (DCS) is normalized on the absolute scale using the relative flow method, with Ar as a reference gas. The theory is obtained with IAM+SCAR method (Independent Atom Model + Screening Corrected Additivity Rule). Experiment and theory are generally in very good agreement, considering absolute scale and shape.

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Experimental and Theoretical Momentum Distributions of Molecules with Astrochemical Relevance

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Synopsis. Electron momentum spectroscopy has been used to study the electronic structure of two molecules of astrochemical relevance: benzonitrile and propylene oxide. The experimental electron binding energy and momentum distributions for the outer valence molecular orbitals are compared to theoretical predictions using outer valence Green's Function and density functional theory methods with the aug-cc-pVTZ basis set. The agreement between experiment and theory is generally good.

Advances in instrumentation and detection technologies have led to an increasing number of molecules being identified in the interstellar medium (ISM). More than 320 molecules have been detected in the ISM, as of September 2024¹. Both benzonitrile (C₆H₅CN) and propylene oxide (C₃H₆O) are within this number. The chemical reactions to synthesize molecules in the ISM from smaller precursor atoms and molecules range from well known reactions to very unusual processes².

A molecule's reactivity is largely governed by its electronic structure. Electron momentum spectroscopy (EMS) has become a powerful technique to measure the valence electronic structure of molecules, yielding the electron binding energy and momentum distribution for individual molecular orbitals³. EMS studies have led to an improved understanding of the relationship between electron momentum distribution and chemical reactivity⁴.

The valence molecular orbitals of benzonitrile and propylene oxide have been measured with EMS. Corresponding theoretical predictions of the momentum distributions were performed via DFT methods, with the ω B97X-D functionals and aug-cc-pVTZ

basis, at the equilibrium geometry and also including molecular vibrations. Binding energies were predicted using the OVGF/aug-cc-pVTZ level at the optimised geometry.

The agreement between momentum distributions obtained by experiment and theory is good, with the majority of molecular orbitals showing similar shapes and structure.

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Radiation Damage to DNA Nanostructures: From Fundamentals to Applications

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Synopsis. The talk overviews our recent experiments irradiating DNA origami nanostructures with ionizing particles. Folded DNA nanostructures exhibit enhanced resistance to ionizing radiation enabling their use in single-molecule studies of radiation effects on DNA. Except for this fundamental research, DNA origami can be used in many applications ranging from targeted drug delivery, through lithography to digital data storage. Particular attention will be given to our recent studies related to the last mentioned, exploring the radiation effects on data-carrying DNA nanostructures.

Even though the DNA is highly stable under certain conditions, ionizing radiation represents an effective means of its damage. Over the last decade, we have used a range of techniques to study the radiation damage to DNA, ranging from fundamental studies of DNA building blocks [1] to plasmid DNA in solution.[2] A unique approach for studying damage to precisely defined DNA sequences represents single-molecule experiments with DNA origami nanostructures (DONs).[3] To explore the possibilities for using this technique in experiments with ionizing radiation, we first explored the radiation effects on the bare DONs, demonstrating their enhanced stability in comparison to supercoiled plasmid DNA.[4] This enabled further studies of the radio-sensitizing effects of chemical modifiers on DNA sequences.[5] While resistive to indirect effects of IR such as OH radical damage, DONs remain sensitive to direct radiation effects, which can be used to shape the DONs for applications. [6] Recently, we became a part of the NEO consortium (neodna.eu) exploring novel ways for DNA-based memories. DNA-based memory can solve many challenges of current digital data storage such as the limited

capacity of the conventional media or its short lifetime. With an aimed high density of data, however, the natural ionizing radiation becomes an issue. Even a single ionizing particle passing through the nanostructure can cause large data losses, which cannot be corrected during the data reading. The experiments that will be presented aim to evaluate the radiation effects on such data-carrying nanostructures and optimize their design to ensure the desired data preservation capabilities.

We acknowledge the support of the European Union via project number 101115317 and the COST action CA20129 Multichem.

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Importance of Radiation Induced Foci (IRIF) in Radiation Research and Health Science

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Synopsis. This work explores the effects of ionizing radiation (IR) on DNA, specifically double-strand breaks (DSBs), which can lead to cell death and cancer. Understanding DSB repair mechanisms is crucial for cancer treatment, space missions, and nuclear safety. Using advanced imaging techniques, the study examines how cells form repair complexes within specific chromatin environment and radiation influences the whole chromatin in the cell nucleus as a system. Findings reveal that chromatin reorganization at DSB sites influences the formation of repair complexes, allowing cells to efficiently choose the best repair strategy. Additionally, changes in pannuclear chromatin architecture post-irradiation are characteristic for cell types and potentially linked to cellular radioresistance, with distinct differences observed between healthy and cancer cells in their ability to restore pre-irradiation chromatin structure. Overall, the research underscores the role of chromatin as a dynamic system that integrates various factors during DSB repair.

Ionizing radiation (IR) causes breaks in the DNA strand, with double-strand breaks (DSBs) being the most critical type of damage that can result in cell death, mutations, or cancer. Understanding the mechanisms of DSB repair is thus essential, especially concerning cancer development, advancements in radiotherapy, planning manned missions to space (especially to Mars), and addressing the potential risks of terrorist misuse of radioactive materials or warfare.

The effectiveness and precision of DSB repair are influenced by the repair mechanism (nonhomologous end-joining, NHEJ, homologous recombination, HR, and alternative repair pathways), the type of DSB damage, and the location of DSB damage relative to specific chromatin environment. While various factors, such as radiation type, dose, and cell type, are known to

affect the repair process, a key question remains: how does a cell choose a specific repair mechanism for individual DSB sites? ^[1]

Our analysis using high-resolution 3D-confocal microscopy and Single-Molecule-Localization-Microscopy (SMLM) ^[2,3] has shown distinct chromatin reorganization at individual DSB sites, ^[4] which correlates with the ability to form non-homologous end joining (NHEJ) or homologous recombination (HR) repair complexes. ^[5] This indicates that the chromatin structure at DSB sites integrates various factors related to the global cellular state and local radiation damage, allowing the cell to efficiently determine the best repair method. ^[1]

Furthermore, changes in chromatin architecture after irradiation and the geometric characteristics of repair foci have been

linked to post-irradiation cell status and potentially cellular radioresistance,^[6] although the nature of this relationship is still under investigation.^[1]

Finally, we have observed cycles of changes in chromatin architecture in virtual space during DSB repair, revealing differences between healthy and cancer cells in their capacity to restore the original chromatin structure prior to irradiation, suggesting that (pannuclear) chromatin also reacts to irradiation as the whole, functioning thus as a complex responsive system to irradiation.^[4,7]

Methods:

Single Molecule Localization Microscopy (SMLM)^[2-5] is an innovative optic microscopy technique that offers high-resolution insight into cellular structures and processes at the single molecule level, under physiological conditions and without the need for image analysis. SMLM can be advantageously used to study the architecture of chromatin and repair complexes at DSB sites. By enabling precise localization of γ H2AX, 53BP1, RAD51 and further molecules within repair foci, SMLM allows researchers to investigate the spatial organization and temporal behavior of DNA repair proteins, providing a deeper understanding of cellular mechanisms in response to DNA damage. This technique holds significant potential for advancing our knowledge in areas such as radiation biophysics and cancer biology. Combined with confocal microscopy, SMLM allows the study of DNA damage and repair processes at multiscale, which is crucial for understanding them in their whole complexity.

At the microscale, the data (the numbers and various parameters of the repair foci) was studied with the DeepFoci software^[8] developed by us. It is a cutting-edge

software application that utilizes deep learning algorithms to facilitate the rapid and automatic analysis of DNA double-strand breaks induced by ionizing radiation. The software is designed to identify and quantify foci, which are crucial markers for understanding DNA damage and repair mechanisms. By leveraging advanced image processing techniques, DeepFoci enhances the efficiency and accuracy of foci detection, making it an invaluable tool for researchers in the fields of molecular biology and cancer research. Its ability to streamline the analysis process significantly contributes to the understanding of cellular responses to radiation, ultimately aiding in the development of targeted therapies and interventions.

For the analysis of SMLM data, we developed numerous mathematical procedures, e.g. based on persistent homology, as it is described in detail in Weidner et al, CSBJ, 2023.^[3]

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Synthesis and Comprehensive Characterization of TiO₂ Nanoparticles Doped with Cu and Rare-Earth Elements

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Synopsis. Nanostructures of wide band gap semiconductors doped with transition metals and rare earth elements (REEs) exhibit promising applications in biomedicine, military, and aerospace. In particular, specific doping can enable combination of photocatalytic activity and up-conversive feature. Here, we report on synthesis of Cu- and REE-doped TiO₂ nanoparticles by sol-gel, hydrothermal, and extraction-pyrolytic methods. X-ray absorption near-edge structure (XANES) analysis along with Raman spectroscopy, XPS, and SEM-EDX studies provided insights into structural and electronic properties of the doped TiO₂ nanoparticles. Outlook and future perspectives of the engineered nanostructures in catalysis and biomedical fields are comprehensively discussed.

The design and synthesis of TiO₂ nanoparticles (NPs) doped with transition metals and rare earth elements (REE) hold significant importance for applications in biomedicine, military, and aerospace [1, 2]. In this study, TiO₂ NPs doped with Cu and Er, Yb were synthesized using sol-gel, hydrothermal, and extraction-pyrolytic methods.

XANES analysis explored their electronic structure, while Raman spectroscopy showed that hydrothermal and extraction-pyrolytic methods favoured the anatase-to-rutile phase transition at higher temperatures. The phase composition, confirmed by Raman and XPS, is essential for optimizing photocatalytic properties of TiO₂ NPs.

Additionally, incorporating Cu and REEs into TiO₂ NPs not only imparted up-conversion property to them but also improved their visible-light-driven photocatalytic activity crucial for water splitting and antibacterial applications. Scanning electron microscopy (SEM) and energy-dispersive X-

ray (EDX) spectroscopy were employed for structural characterization of the synthesized NPs, confirming a uniform distribution of dopants and identifying morphology differences in the samples caused by fabrication method. Results are compared with theoretical predictions of Density Functional Theory modelling.

The obtained results provide new research-based fundamental knowledge and deep understanding of how different synthesis techniques and dopants affect the properties of TiO₂ NPs. The research was funded by the Latvian Scientific Council grant LZP-2021/1-0464.

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Manipulating Metal Atoms in Clusters and Nanoalloys to Control Catalysis

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Synopsis. *“But I am not afraid to consider the final question as to whether, ultimately - in the great future - we can arrange the atoms the way we want; the very atoms, all the way down! What would the properties of materials be if we could really arrange the atoms the way we want them? They would be very interesting to investigate theoretically. I can't see exactly what would happen, but I can hardly doubt that when we have some control of the arrangement of things on a small scale we will get an enormously greater range of possible properties that substances can have, and of different things that we can do”.*

So wrote Feynman in 1959 and the words are so amazing you never tire of reading them. In fact it was Don Eigler, with his manipulation of atoms in the STM, that made this quotation famous. Yet cluster physics competes favourably in the matter of arranging the atoms, and it is much more scalable than STM – various labs are now envisaging cluster deposition at the gram and even kg scale (as I will show), suggesting real industrial possibilities. And nanoalloys offer even more scope.

In this talk I will survey some recent advances in the quest to arrange the atoms in clusters, and its consequences – as enabled by new experimental production methods, probed by state-of-the-art measurement techniques, like aberration-corrected electron microscopy and photoemission with synchrotron radiation, and manifested in satisfying functional performance. The emphasis will be on supported clusters and alloys of noble metal atoms.

First [1,2], the arrangements and dynamics of size-selected (mainly Au and Pt) clusters, deposited on surfaces, are revealed by time-resolved single-cluster TEM imaging,

and their energetics by the new variable-temperature version of the same method. Secondly, core-level photoemission of these same systems distinguishes smooth screening effects from a size of about 1000 atoms down to 50, while non-scalable quantum effects kick in at smaller sizes. Thirdly, mixing different kinds of atoms (eg Ag and Pd) inside a nanocluster tunes the chemical performance (via the electronic states), as illustrated by photocatalytic transformations of alcohols.

Together, the measurements provide a snapshot of the progress towards realizing Feynman's vision in the world of clusters and nanoalloys.

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Radiation Damage and Thermal Annealing Kinetics of Radiation Defects in CVD Diamond Irradiated by Xe Ions

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Synopsis. The variation in the spectra of diamond optical absorption in a wide range of 1.5–5.5 eV due to the energetic Xe ion irradiation, as well as during a further thermal annealing procedure up to 650 °C of the irradiated CVD diamond samples (from Diamond Materials, Freiburg, Germany), has been studied experimentally. The radiation-induced origin of the defects responsible for several bands has been confirmed and the annealing curves for the radiation-induced defects responsible for the optical absorption around 2 eV, 2.5 eV and 4.1 eV (including vacancies and interstitials) have been experimentally constructed.

Optical and dielectric materials play a key role in numerous high tech applications and attract increasing attention for their modelling from the first principles. In particular, diamond is a very attractive material, not only as a gemstone but also for fundamental science and different innovative applications. Moreover, it is the material addressed in the major future research directions of the EU programme's Quantum Technologies Flagship and Quantum Communication Infrastructure.

In this paper, we study experimentally and theoretically the radiation properties of CVD diamond exposed to swift heavy ions with varying fluence, which is relevant for windows in fusion reactors.

The radiation-induced optical absorption at 1.5–5.5 eV has been analyzed in CVD diamond disks (5 mm diameter samples with thickness 0.4 mm) exposed to 231-MeV ¹³²Xe ions with four fluences from 10¹² to 3.8 × 10¹³ cm⁻². The range of xenon ions was $R = 11.5 \mu\text{m}$. The intensity of sev-

eral bands grows with ion fluence, thus confirming their radiation-induced origin. The recovery of radiation damage has been investigated via isochronal (stepwise) thermal annealing procedure up to 650 °C, while all spectra were measured at room temperature. Based on these spectra, the annealing kinetics of several defects, in particular carbon vacancies (broad band ~2 eV) and complementary C-interstitial-related defects (~4 eV), as well as impurity-related complex defects (narrow bands around 2.5 eV) have been constructed. The experimental kinetics have also been analyzed in terms of the diffusion-controlled bimolecular reactions. The migration energies of tentatively interstitial atoms (mobile components in recombination process) are obtained, and their dependence on the irradiation fluences is discussed.

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Investigation of Radiation Defects by Thermal Annealing of BaF₂ and CaF₂ Crystals Irradiated with Fast Xenon Ions

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Synopsis. In the present work, radiation defects in BaF₂ and CaF₂ crystals are investigated upon irradiation with 220 and 230 MeV ¹³²Xe ions to fluences of 10¹¹-10¹⁴ ions/cm². The optical absorption spectra were measured in the range from 10 to 1.5 eV. To investigate the thermal annealing of color centres created in BaF₂ and CaF₂ single crystals, step-by-step annealing of radiation defects was carried out. The 9.7 eV band in CaF₂ is of a hole nature, and its growth starts at the destruction of the 6.5 eV band, which is a V₂ center representing the F₃⁻ fluorine quasi-molecule. In the UV region of the spectrum of BaF₂, a slight increase in the 9.18 eV band is observed in the temperature range 450-575K, which is accompanied by a decrease in the bands with maxima of 6.5 and 8.2 eV, that is, the latter is also of hole nature.

BaF₂ crystals possess high radiation resistance and are used as scintillators with high time resolution in high-energy physics. BaF₂ crystals are characterized by fast synchronization due to a very short decay time of about 0.8 ns of luminescence at 195 and 220 nm. CaF₂ crystal also has relatively high radiation resistance. This property allows the use of the crystal and BaF₂ in scintillation detectors. The current study aims to explore the processes involved in the formation of defects in BaF₂ and CaF₂ crystals when they are exposed to ¹³²Xe swift heavy ions. This will be done using optical absorption spectroscopy across a wide spectral range, from vacuum ultraviolet to near-infrared spectral region. Additionally, the absorption spectra will be analyzed through sequential thermal annealing.

BaF₂ single crystals from Epic Crystal (China) and CaF₂ single crystals (S. V. Vavilov GOI, Russia) were used in this work. BaF₂ and CaF₂ crystals were irradiated with ¹³²Xe ions at a DC-60 cyclotron (Astana, Kazakhstan). Radiation parameters

of xenon ions in BaF₂ and CaF₂ crystals calculated using the SRIM code. It has been discovered that the range for xenon ions is almost the same ~18 μm, the same can be said about the electronic and nuclear energy losses of ions. The ratio Se./Sn, ≈ 300, i.e., electronic losses dominate [1].

Absorption spectra were measured using a Jasco V-660 dual-beam spectrophotometer and a VMP-2 vacuum diffraction monochromator. Step-by-step annealing of radiation defects was carried out to study the thermal annealing of the color centers. Multiple heating-cooling-measurement cycles were performed under identical conditions with an increase in annealing temperature (T_{ann}) by 20-30 K. All spectra were measured at room temperature.

From the analysis of fluence-dependent absorption spectra, it is observed that the defect concentration increases as the fluence increases. In the absorption spectra of irradiated crystals, non-identifiable color centers are present. The concept of color centers developed for alkali-halide crystals (AHC) was utilized to analyze

defects. To analyze the absorption spectra of BaF₂ and CaF₂ crystals before and after annealing, we used the scheme of defects in KBr crystal, which is a typical representative of AHCs. An impurity-free and defect-free KBr crystal has absorption only in the ultraviolet (UV) and infrared (IR) regions of the spectrum. After irradiation, absorption of color centers is created between these regions. In region (UV), color centers are of hole nature. In region (IR) defects are electronic.

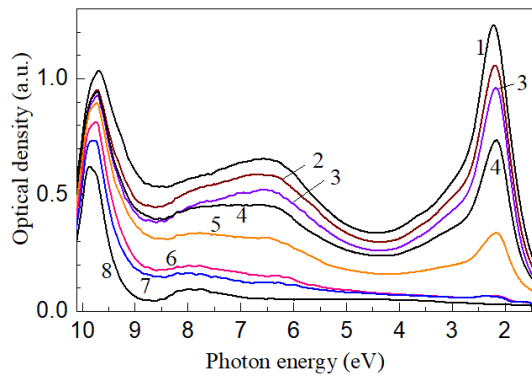


Figure 1: Optical absorption spectra of CaF₂ single crystals after irradiation with 230 MeV ¹³²Xe ions to fluence $\Phi = 5 \times 10^{13} \text{ cm}^{-2}$ and step-by-step annealing in the temperature range (440-1023K) 1 - after irradiation; 2 - 440 K; 3 - 470 K; 4 - 500 K; 5 - 540 K; 6 - 580 K; 7 - 660 K; 8 - 773 K; 9 - 1023 K

Upon analyzing Figure 1, it has been determined that the 9.7 eV band in CaF₂ exhibits hole-like characteristics and starts to emerge when the 6.5 eV band, representing a V₂ center analogous to a quasi-molecule of fluorine F₃⁻, breaks. Accordingly, the 9.7 eV band may be due to more complex hole aggregates. The center responsible for the 8.15 eV band also has a hole nature and a structure close to the 6.5 eV center. In the UV region of the BaF₂ spectrum (Fig. 2), a slight increase in the 9.18 eV band is observed in the temperature range of 450-575K. This increase is accompanied by a decrease in the bands with maxima of 6.5

and 8.2 eV, indicating a hole nature for the latter.

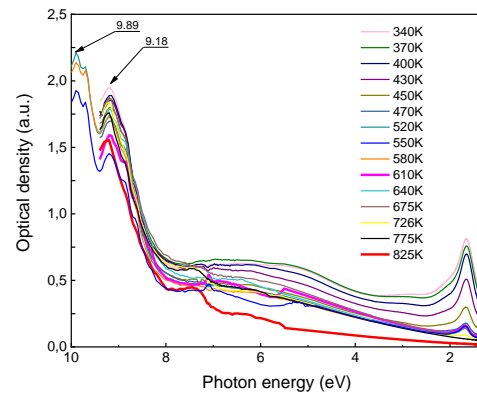


Figure 2: Optical absorption spectra of BaF₂ single crystals after irradiation with 220 MeV ¹³²Xe ions to fluence $\Phi = 1 \times 10^{14} \text{ cm}^{-2}$ and stepwise annealing in the temperature range (340-825 K).

The bands at 7.4 eV, 2.24 eV, and 3.04 eV remain nearly unchanged across the entire range of annealing temperatures. The temperatures at which color centers of different types are thermally destroyed were also determined. one selected referencing style.

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Perspectives on Electrochemical Chemosensing

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Synopsis. Electrochemical chemosensing is essential for advancing diagnostics, especially in point-of-care (PoC) technologies. We present two primary architectures: planar PCB-based graphene field-effect transistors (GFETs) and microneedle-based biosensors. Planar GFETs, fabricated on printed circuit boards using scalable spray-coating techniques, detect pH and sodium ions (Na^+) at clinically relevant ranges for less than \$0.25 per device. Building on this platform, GFETs were integrated onto polycarbonate microneedles, enabling continuous, minimally invasive health monitoring through interstitial fluid sampling. These microneedle sensors, developed via laser lithography and spray-coating, demonstrate a novel approach to wearable biosensors. The combination of affordability, scalability, and the versatility of graphene paves the way for potential future PoC diagnostic systems.

The growing demand for scalable, cost-effective biosensors has driven the development of advanced electrochemical sensing platforms.[1] This surge in demand is largely fuelled by the healthcare industry's shift towards decentralized, personalized medicine and the need for rapid, accurate diagnostics in various settings, from hospitals to homes. [2] GFETs, a central focus of our ongoing research, have emerged as a promising solution by harnessing graphene's exceptional electronic properties and processability. [3] Graphene's unique characteristics, including its high carrier mobility, large surface-to-volume ratio, and chemical stability, make it an ideal material for sensing applications. [4] Our work has culminated in the development of two distinct architectures on planar and microneedle substrates. These platforms represent significant advancements in the field, each offering unique advantages and applications in the realm of chemical and biological sensing.

Our team designed planar GFETS on printed circuit boards (PCBs) using sprayable graphene inks. [5] These devices detect sodium (Na^+) and monitor pH with a

sensitivity of 131 μA per $\log_{10}\text{Na}^+$ and 143 μA per pH, respectively. The Lab-on-PCB platform, enabled by electrolyte gating, provides real-time electrochemical monitoring in aqueous solutions. Manufactured using scalable PCB processes, these devices are designed to meet the stringent cost and sensitivity requirements of point-of-care (PoC) diagnostics, achieving production costs of less than \$0.25 per sensor.

Building on this, our research has extended the GFET platform to microneedle-based biosensors, aimed at enabling continuous, minimally invasive health monitoring.[6] Using a combined spray-coating and photolithography process, we fabricated GFETs on the complex non-planar surface of polycarbonate microneedles. This setup allowed us to pattern graphene channels as small as 67 μm in length while optimizing their electrochemical performance by monitoring resistance during fabrication. These microneedle sensors, characterized through SEM and EDX mapping, exhibit ambipolar modulation in solution, paving the way for real-time detection of biomarkers in interstitial fluid.

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Effect of Irradiation with Swift Heavy Ions on Luminescence of CsI:Tl Crystals

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Synopsis. CsI:Tl scintillation crystals are widely used in nuclear and high-energy physics experiments. In the present work, the luminescent properties of CsI:Tl crystals induced by 230 MeV ¹³²Xe ions to fluences (1×10^{11} - 1×10^{14} ions/cm²) at 295K (accelerator DC-60, Astana, Kazakhstan) have been studied and analysed. The study was carried out by optical absorption and luminescence spectroscopy, as well as time-resolved optically stimulated luminescence. The surface was examined by atomic force microscopy. The intensity of the 553 nm scintillation luminescence band and its light output were found to decrease with increasing fluence. The conversion efficiency for the studied samples is independent of fluence. Thus, radiation damage does not affect the conversion efficiency of the CsI:Tl crystal. The formation of tracks does not reduce the conversion efficiency of the CsI:Tl crystal, but tracks participate in the scintillation process, in the form of energy reabsorption from Tl⁺ -centers, which leads to the degradation of the light output.

Typically, CsI:Tl is used to detect ionizing radiation, particularly ions and fission products. The development of large-area silicon photodiodes, whose quantum efficiency corresponded to the CsI:Tl spectrum, strongly stimulated the use of this crystal in nuclear physics experiments. The fabrication and application of large detector arrays is limited by radiation damage to the scintillation materials. In general, radiation damage creates color centers that reduce transparency, destroy luminescent centers in the material, or prevent their formation. Therefore, it is very important to know the behavior of luminescent materials in strong radiation fields.

The aim of this work is to study and analyze the luminescent properties of CsI:Tl crystals irradiated with swift heavy xenon ions with fission fragment energies depending on the fluence using optical spectroscopy and atomic force microscopy.

CsI:Tl single crystals of ALINEASON (Germany), were used in the study. The crystals have a cubic structure of CsCl. The samples had dimensions of 5×5×0.5 mm. The concentration of thallium was 0.5%. The samples underwent irradiation on a DC-60 accelerator with 220 MeV ¹³²Xe ions to fluences ranging from 10¹¹ to 10¹³ cm⁻² at 300 K. The radiation parameters of the 230 MeV ¹³²Xe ion in CsI:Tl crystals were calculated using the SRIM code. The ratio of S_e (electronic energy loss) to S_n (nuclear energy loss) is 265, meaning that ionization losses dominate, and predominantly electronic excitations create radiation defects. The ion range is R = 24.76 μm.

Optical absorption spectra were measured using a T8DCSIS19-2 dual-beam spectrophotometer (China) in the spectral range of 190-900 nm. Photoluminescence and excitation spectra were measured on a SM2203 Solar universal spectrofluorimeter (Belarus). The wavelength range is from 220 to 920 nm. Luminescence attenuation

kinetics were measured using a Laser Ekspla NT ns tunable laser system (2708122) with a pulse duration of 7 ns (Vilnius, Lithuania). The surface morphology of CsI:Tl samples was investigated by atomic force microscopy using an AIST-NT SmartSPM microscope

The whole spectral range studied is primarily characterized by the well-known scintillation band at 553 nm (2.24 eV) of the Tl^+ center and the emission band of self-trapped excitons (STE) at 340 nm (3.65 eV). With increasing fluence, PL intensity and the luminous yield of this center's luminescence decrease. It should be noted that it is a known fact that the effect of radiation on CsI:Tl crystals leads to the deterioration of their scintillation parameters. The light yield decreases nonlinearly with increasing fluence. It can be argued that the degradation of the light output is not associated with a cardinal deterioration of the transparency of the crystal, which remains practically transparent in the same spectral range before and after irradiation to different fluences. In the process of ion irradiation, the crystal is heated up to $T \geq 330K$. At such high temperatures, the color centers are no longer stable due to thermal ionization, so the CsI:Tl crystal turns out to be extremely resistant to irradiation.

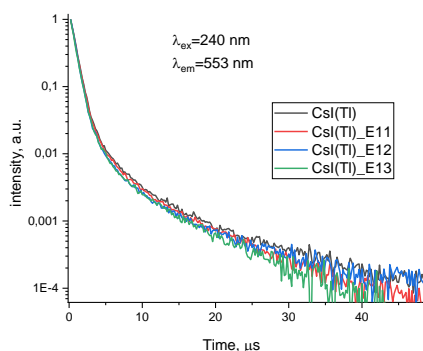


Figure 1 Decay of 553 nm luminescence in crystals as a function of fluence. Excitation was carried out by a laser pulse with a wavelength of 240 nm.

The conversion efficiency for the studied samples is independent of fluence. This means that in the scintillation pulse, which is registered before and after ion irradiation, the CsI:Tl crystal emits the same number of photons, i.e. radiation damage does not affect the conversion efficiency of the CsI:Tl crystal (Fig.1). The blurring of kinetics at the end of the process likely results from interacting with defects. At irradiation with swift heavy ions the degradation effect can be caused by macro-defects (hillocks on the surface and tracks).

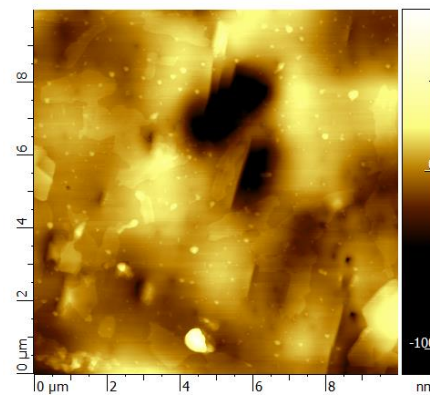


Figure 2 AFM images of CsI:Tl crystals irradiated with 230 MeV ^{132}Xe ions to a fluence of $1 \times 10^{13} \text{ cm}^{-2}$ at 295K. in 3D format

Due to the creation of tracks and overlapping of tracks, the space for free motion of electron excitation is sharply narrowed, which leads to a decrease of STE, and at the creation of Frenkel pairs of defects, they will annihilate due to the impossibility of scattering. These defects do not reduce the conversion efficiency of the CsI:Tl crystal but participate in the scintillation process in the form of energy reabsorption from Tl^+ centers.

Acknowledgments

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Analysis of Self-Trapped Hole Mobility in Alkali Halides, Alkaline-Earth Halides and Other Binary and Complex Metal Halides

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Synopsis. The small radius hole polarons (self-trapped holes (STH) known also as the V_k centers) are very common color centers observed in numerous alkali halides and alkaline-earth halides. Their mobility controls the rate of secondary reactions between electron and hole defects and thus radiation stability/sensitivity of materials. We have analysed here the correlation between the temperatures at which hole polarons start migration in a series of alkali halides (fluorites, chlorides, bromides, iodides) and the lattice displacement around quasi-molecule. These results are especially important for identification of the self-trapped holes, for example, in novel scintillating materials such as SrI_2 and CaI_2 , as well as in a large family of perovskite halides ($KMgF_3$, $BaLiF_3$ etc) and more complex halide materials

The mobilities of small radius polarons affect properties of many insulating materials and thus attract considerable attention. The self-trapped hole (STH) polarons (called V_k centers), in which a hole is shared by two nearest halogen ions, X_2^- , are very common color centers created in alkali halides, alkaline-earth halides and some other halides under various kinds of irradiation (UV light, electrons, gamma rays, neutrons, heavy swift ions) [1, 2 and references therein] Their mobility controls the rate of secondary reactions between electron and hole defects and thus radiation stability/sensitivity of materials.

The hole polarons start to migrate and recombine above certain onset temperatures (in the range 50–200 K). Their diffusion-controlled decay has been observed by different experimental techniques in almost all alkali halides, as well as in some other binary halides, but also in complex halides, such as perovskite halides, ammonium halides, halide sodalites etc.

In this paper, we review and analyse the STH migration temperatures for a series of

alkali halides as a function of halogen-halogen (X-X) distance in a regular crystalline lattice as well as the bond length in isolated X_2^- molecular ions. A simple linear dependence of the migration temperatures of self-trapped holes in several classes of ionic solids was established as a function of the two halogen atom displacement constituting the X_2^- quasi-molecule from the regular lattice sites [2]. As demonstrated, this correlation allows us to identify the STH and their structural configuration in various cases, including the promising scintillating material SrI_2 and CaI_2 .

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Photodissociation of Molecular Ions Relevant for Astrochemistry and Laboratory Investigation

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Synopsis. In this contribution, we explored the mechanisms of photodissociation in non-symmetric systems that consist of hydrogen, helium, alkali alloys, ions, and molecular ions. Quantum mechanical analysis of the cross-sections and spectral rate coefficient data has been performed. The obtained results have potential laboratory and astrophysical applications.

One can note the current importance of the investigation of optical properties of various small molecules and corresponding atomic and molecular data [1]. Recent experimental and theoretical advances in the field of molecular astrophysics, astrochemistry and atmospheric science have allowed new results to be obtained. Data and database related to processes involving these molecules have become increasingly important for developing models and simulations of complex physical/chemical processes. Recently, the Leiden VUV cross section database specialised for photodissociation and photoionization of molecules of astronomical interest has been updated with both new astrophysically relevant molecular species and a brief review of the basic physical processes [2]. Also, these data are becoming more and more crucial for analysing observations and results of measurements in various fields [3].

Here, we study the photodissociation processes in non-symmetric systems comprising alkali atoms, ions, molecular ions, hydrogen, and helium. As one of the main components of He/H plasma sources, such as synchrotron devices, high voltage glow discharges, inductively coupled plasma generators, capacitively coupled RF discharges, and magnetically confined plasmas, it has been found that the ionic helium

hydride molecule plays a unique role in the current development of thermonuclear fusion. The alkali hydride species, both ionic and neutral, are critical for understanding how the molecular universe was formed and evolved [4]. Even though they are involved in several astrophysical and astrochemical processes, including radiative transfer, little is known about their spectroscopy in terms of theory and observation, particularly with regard to molecule ions. The calculated photodissociation data of some molecular ions have been reported.

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Some Experimental Insights into the Microphysics of Ice Processing by Cosmic Rays

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Synopsis. We present a dedicated experimental study of microscopic mechanisms controlling radiolysis and sputtering of astrophysical ices due to their bombardment by cosmic ray ions. Such ions are slowed down due to inelastic collisions with bound electrons, resulting in ionization and excitation of ice molecules. In experiments on CO ice irradiation, we show that the relative contribution of these two mechanisms of energy loss to molecule destruction and sputtering can be probed by selecting ion energies E_{ion} to be near the peak of the electronic stopping power $S_{\text{el}}(E_{\text{ion}})$. We have observed a significant asymmetry, both in the destruction cross section and the sputtering yield, for pairs of ion energies corresponding to same values of the stopping power on either side of the peak. This implies that the stopping power does not solely control these processes, as often assumed in the astrophysical literature. Our results suggest that electronic excitations represent a significantly more efficient channel for radiolysis and sputtering of CO ice.

We show that the scaling dependencies on the electronic stopping power, often used in the literature to describe the sputtering yield and destruction cross section of ice molecules, clearly break down near the peak of $S_{\text{el}}(E_{\text{ion}})$. The measured destruction cross section of CO deviates from the predicted $\sigma_{\text{des}} \propto S_{\text{el}}^{1.5}$ dependence, showing a significant enhancement at ion energies below the peak. A similar, but less significant deviation from the $Y \propto S_{\text{el}}^2$ dependence is observed for the sputtering yield. These results suggest that among the two contributions to the electronic stopping power – ionization and electronic excitations – the latter is a notably more efficient channel for CO radiolysis. The same conclusion may certainly be correct for CO sputtering, too.

To the best of our knowledge, the reported experiments [1] are the first dedicated attempt to explore the relative importance of the excitation and ionization channels in the CR processing of astrophysical ices. In a separate publication [2], we will report on detailed analysis of the radiolysis chemistry driven in the discussed experiments.

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Ion Processing of Astrophysically Relevant Molecular Systems

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Synopsis. Understanding the origin and evolution of primitive organic in space is fundamental, since extraterrestrial organic matter delivery through meteoroids and comets is one of the possible sources of organic matter available at the early Earth. Molecular systems in space are exposed to energetic ions (e.g. solar wind, ions trapped in magnetospheres or cosmic rays). During my talk, I will present examples of intra-cluster molecular growth processes triggered by ion collisions and ion processing of astrophysical ice analogues performed at the ion beam GANIL facility (Caen, France).

“Where do we come from” is one of the important fascinating open questions of science and philosophy. How did life emerge, what is the origin of organic matter in the universe? Complex organic molecules have indeed been observed in space (e.g.: comets, meteorites, asteroids, molecular clouds).

In space, the molecular matter is energetically processed by ionizing radiation and two scenarios are proposed to explain the emergence of new molecular species. On the one-hand, the *bottom-up* approach proposes the growth of larger molecules from smaller subunits. On the other hand, the *top-down* scenario considers the emission of molecular species from a large piece of matter. In order to study the processes leading to the formation of complex organic molecules, we have considered ion interaction with molecular clusters or icy mantels.

During my talk, I will present an overview of experimental studies performed at ion beam GANIL (*Grand Accélérateur National d'Ions Lourds*) facility (Caen, France) leading to molecular complexification within molecular clusters induced by low-energy ion collisions: (i) intra-cluster molecular growth processes in clusters of

polycyclic aromatic hydrocarbons or fullerenes triggered by knock-out processes [e.g.: 1-3]; (ii) formation of peptide bonds in collisions of a single He²⁺ ion with amino acid β -alanine clusters [4]. I will also present the examples of ion processing of astrophysical ice analogues and condensed complex organic molecules [e.g.: 5].

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Ongoing Investigation of Ice Analogs of the Solar System Icy Moons using Laboratory Facilities.

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Synopsis. The aim of the study is to provide new insight on the properties of molecular oxygen and mixtures with H₂O, CO₂, N₂, CH₃OH, CH₄, exploring temperatures from 8K to 80 K to further constrain the nature of the observed features on the Galilean satellites. Experiments have been performed in the vis range using the AU-UV beam line of the ISA ASTRID2 ring storage, at the University of Aarhus.

Spectroscopy in the visible and near-infrared allows investigating surface composition, thanks to the several diagnostic features due to H₂O, CO₂, nitrogen-rich organics and nitriles, as an example. Molecular oxygen in its solid form has been detected on the surfaces of Ganymede, Europa, and Callisto via telescopic observations. Ground-based observations, in particular, revealed two distinct features at 577.3 nm and 627.5 nm, which were attributed to solid O₂ on Ganymede's trailing hemisphere [1]. These same features were later detected on Europa and Callisto [2], and more recently, re-observed on Europa and Ganymede with higher contrast, allowing clearer identification on Europa as well (Spencer J., personal communication). The observed features are recognized to be the result of a double electronic transition of two adjacent O₂ molecules [3, 4]. However, the origin and persistence of molecular oxygen on icy surfaces like those of the Galilean moons remain debated. If O₂ is primordial, mechanisms must exist to

effectively trap it within the water ice layers. On the other hand O₂ in its solid phase must be constantly replenished through radiolysis to compensate for its depletion due to desorption. Despite these hypotheses, it is still debated how O₂ can be trapped and sustained on the surfaces of the icy satellites of the outer solar system planets. Laboratory experiments on ice analogs to the surfaces of the icy moons of Jupiter and Saturn can help address this open question. The same data would be of interest to study the surface composition of icy moons of Saturn, Uranus and Neptune, properly scaled to the thermal and ionospheric environments at these solar distances.

Our purpose is to provide new insight on the properties of molecular oxygen and mixtures with H₂O, CO₂, N₂, CH₃OH, CH₄, exploring temperatures from 8K to 80 K to further constrain the nature of the observed features on the Galilean satellites. Experiments have been performed in the vis range using the AU-UV beam line of the

ISA ASTRID2 ring storage, at the University of Aarhus.

In this work we summarize measurements obtained in four runs in 2019, 2022 [5], 2023, and 2024 and a comparison with the Ganymede and Europa observations.

The proposed measurements allow building a background for the future interpretation of data acquired with the MAJIS instrument [6] on board the ESA JUICE mission.

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Radiation Processing of Interstellar Ice Analogues

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Synopsis. Radiation processing is one of the main drivers of chemical complexity in space throughout the planets and star formation process. In this talk, I will review some of the recent work carried out at European large-scale facilities in the field of laboratory astrochemistry. Emphasis will be given to projects aimed at understanding the formation of building blocks of life in space.

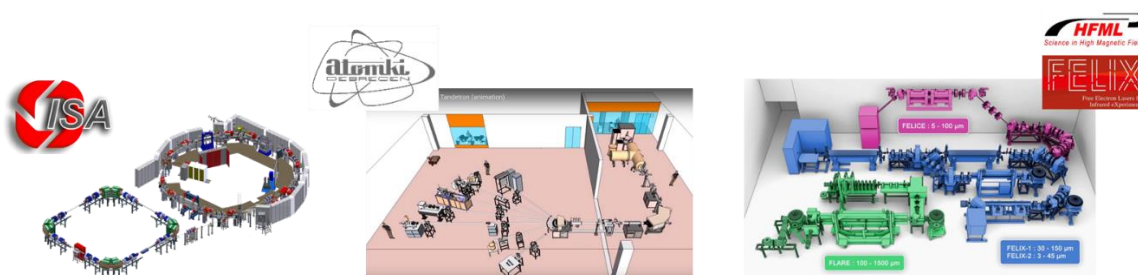


Figure 1. Left: ISA, Centre for Storage Ring Facilities, Aarhus, Denmark. Center: Atomki, Institute for Nuclear Research, Debrecen, Hungary. Right: HFML-FELIX, High Field Magnet Laboratory and Free-Electron Lasers for Infrared eXperiment, Nijmegen, Netherlands.

Complex organic species are expected to be formed in a variety of interstellar environments at the surface of ice grains by means of a combination of energetic and nonenergetic processing, such as photons, electrons, ions, and atoms. However, to date, many fundamental questions on the physicochemical origin of the molecular complexity observed in space by the ground-based Atacama Large Millimeter/submillimeter Array (ALMA) remain unanswered [1-3]. The recent scientific achievements of the spaceborne James Webb Space Telescope (JWST) are marking the onset of a new era for space science, astrophysics, astrochemistry, and astrobiology [4]. The unprecedented combination of JWST and ALMA is currently mapping and characterizing the ice and the gas content of the interstellar medium toward a variety of space environments and physicochemical conditions, revolutionizing our understanding of

the star formation process [5,6]. European large-scale experimental facilities can provide users with unique tools to correctly interpret observations and guide future work (see Figure 1). I will present some of the latest laboratory results on the formation and survivability of key prebiotic species relevant to the origin of life on Earth. I will also discuss how laboratory work can help address some current “Grand Challenges” in astrochemistry.

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Ion-Impact Studies with Astrochemical Relevance

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Synopsis. A large variety of processes can occur in ion-matter collisions. In this work, we examine the specific characteristics of ion bombardment in comparison with the physical and chemical changes induced by photon and electron impact. We focus on the processes taking place in cold environments, primarily in astrophysical ice analogues, but we also consider collisions with gas-phase materials, particularly with gases that make up the studied ices.

Radiation is considered as an important agent of molecular formation in space environments. Laboratory simulations by photon, electron and ion impact on astrophysical ice analogues have demonstrated a large variety of chemical processes including the synthesis of complex molecules [1].

Monoenergetic photon impact is the most selective method to identify the energetic conditions for specific chemical processes. Experimental simulations of natural processes by charged particle impact are more complicated to interpret. It is important to realize that the scenario of ion-matter interaction is very rich. Ion species range from protons to heavy atoms and molecules, anions and cations with different charge states. Their energies span from the few-kelvin thermal region to enormous energies of cosmic rays. Even in single collisions of few-keV-energy small ions with atoms, the number of possible one-electron transitions is very large (target and projectile excitation or ionization, electron transfer, all to a multitude of final states). The number of possible outcomes gets enormously large when stronger perturbation

opens the channels for multi-electron transitions. Collisions of molecular species makes the scenario obviously more complicated. In condensed matter, e.g. in astrophysically relevant ices, secondary electrons and ions regularly create subsequent collisions. Moreover, the stopping of each ion has a history, as different collision mechanisms dominate the different parts of the trajectory.

In the present work we consider the features of ion-impact on ices from the chemistry point of view. It is not a review of a subfield of radiation chemistry of ices, more a search for some specific features and concepts there, with emphasis on the most abundant radiation conditions in space. The work is based on the laboratory simulation experience of our group (e.g., [2]).

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Laboratory Studies on the Radiation-Driven Chemistry in Ices in Space

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Synopsis. Laboratory experiments on the irradiation of astrochemical ice analogues are a key method by which the chemistry of space environments can be better understood, along with the rich inventory of molecules to which this chemistry leads. In this talk, I shall give an overview of experiments carried out recently at the HUN-REN Institute for Nuclear Research on the radiation chemistry and physics of interstellar and outer Solar System ice analogues.

The chemical processing of ices in the dense interstellar medium is known to be a source of complex organic molecules that are important for the development of planetary systems and the emergence of life [1]. The ubiquity of ionising radiation in the form of galactic cosmic rays and stellar winds in these environments means that the radiation-processing of interstellar ices is among the most prominent source of new molecules in space. Such radiation-driven processes are also thought to be of great importance on the surfaces of outer Solar System bodies, such as the icy moons of Jupiter, comets, and Kuiper Belt Objects.

In this talk, I shall present recent results from our laboratory at the HUN-REN Institute for Nuclear Research (Atomki) in Debrecen, Hungary. The talk will begin with an overview of the laboratory facilities at Atomki [2,3], before going on to describe the results of specific experiments. A key theme of this talk in particular will be the so-called survivability of molecules under cosmic ionising radiation, which is important when considering the molecular

inventory of astronomical environments and their prebiotic potential.

Results from the irradiation of amorphous and crystalline astrochemical ice analogues with energetic electrons will be presented, using CH₃OH and N₂O ices as case studies. The results demonstrate that the irradiation-induced decay of the crystalline ices is slower than that of the corresponding amorphous ones due to the stronger intermolecular interactions that must be overcome during the irradiation of the former [4].

The talk will then continue with a discussion on experiments carried out to assess the electron-induced radiolytic destruction of N₂O at different temperatures relevant to the outer Solar System. Our results demonstrate that higher temperatures are more conducive to the radiolytic destruction of N₂O; however, the yield of key radiolytic products exhibit distinct and complex relationships with temperature. These results will be discussed in detail, as will be their implication for nitrogen-based chemistry in the outer Solar System.

Lastly, the talk will conclude with a description of the differences in the results obtained when performing the irradiation of ices using different charged particles. In particular, the proton and electron irradiations of CH₄:H₂O mixed ices will be discussed as a case study [5], and the implications on the chemistry of space environments will be discussed.

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Low (10 K) and High Temperature (10⁴ K) Astrochemistry

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Synopsis. Extreme conditions are recreated on planet Earth to understand the physico-chemical nature of astro-molecules. The astrochemical conditions range from the low-temperature icy mantles (10 K) to high temperature (10000 K) processes. So in the evolution of molecules of life leading to the *Origin of Life* - which extreme condition shall we consider, 10 K or 10000 K?

In the latter part of the 20th and the beginning of this Century several space missions explored icy satellites in our solar system for the first time. All of these icy bodies have revealed a more complex chemistry than expected. Amongst the icy satellites such as Ganymede, Europa, Dione, Rhea, Callisto and Titan are embedded in their respective planetary magnetospheres and hence their surfaces are irradiated by a wide range of energetic ions as well as solar photons both of which release many secondary electrons. UV photons, ions and electrons have all been shown (in the laboratory) to facilitate molecular synthesis. Such energetic processing of simple molecules within ices (10 K) has been shown to synthesise quantum dots / graphene and complex molecules such as amino acids, sugar and even di-peptide links. However, another process by which molecules may be formed is by impacts and shocks.

The observation of large scale craters on the surface of the icy satellites reminds us of the role of impact processes in planetary and lunar evolutions whilst many cometary bodies appear to be the result of collision of

constituent bodies. Such impacts release significant amounts of energy and therefore may provide pathways for large scale molecular synthesis. Indeed it is important to recall that all planetary and lunar surfaces are constantly bombarded by micrometeorites. However, such impacts and the impact associated with shock processing of molecules in extreme conditions largely remains unexplored. In this talk, we will discuss the results of a new experimental programme where elements (their mixtures), molecular ices and mixtures of prebiotic molecules (e.g. amino acids / nucleobases / fatty acids) are subjected to astrochemical impact conditions. The results are intriguing, revealing the formation of minerals, complex molecule synthesis and complex macroscale structures.

Reactive collisions of small aromatic compounds with atoms/radicals by the crossed molecular beam technique

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Synopsis. In our laboratory, we study bimolecular reactions between atomic species and hydrocarbons using the crossed molecular beam method with mass spectrometric detection. A radio-frequency discharge beam source generates atomic and diatomic radicals for precise investigation. Recently, we have focused on the reactions of atomic oxygen, O(³P) and atomic nitrogen, N(²D), with small aromatic compounds like benzene, toluene, and pyridine. These reactions are relevant to energy production, interstellar chemistry, and Titan's atmosphere, with potential implications for prebiotic chemistry. Our experimental results are supported by *ab initio* calculations and statistical models to clarify reaction mechanisms and product distributions.

In our laboratory, we have pursued a systematic investigation of bimolecular reactions involving atomic species and hydrocarbons by means of the crossed molecular beam method with mass spectrometric detection (see, for instance, Ref. 1) for many years. Advantage has been taken of an efficient, versatile radio frequency discharge beam source to produce atomic (C, N, O, S, Cl) and diatomic (CN, OH, C₂) radicals.²

In this lecture, I will present recent results obtained in our laboratory on the reactions involving either atomic oxygen in its ground electronic state, O(³P), or atomic nitrogen in its first electronically excited state, N(²D), with small aromatic compounds (benzene, toluene, pyridine). The investigated systems are of relevance in energy production processes, in the chemistry of the interstellar medium and in the chemistry of the upper atmosphere of Titan, the giant moon of Saturn, with potential implications in prebiotic chemistry.

In all cases, the interpretation of the experimental results has been assisted by dedicated *ab initio* calculations of the underlying potential energy surface and statistical

estimates of the product branching fractions.³⁻⁷

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A Systematic IR and VUV Spectroscopic Investigation of Ion, Electron, and Thermally Processed Ethanolamine Ice

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Synopsis. To investigate the stability and survivability of ethanolamine (EtA) molecules in astronomical environments, we have exposed EtA-containing ices to electron, ion, and thermal processing, under controlled laboratory conditions. Infrared (IR) and vacuum ultraviolet (VUV) spectra were collected at different doses of irradiation. The column density of EtA is demonstrated to undergo exponential decay, and the corresponding half-life doses are obtained. The results show that EtA mixed in H₂O ice is more stable than in pure form and it should survive throughout the star and planet formation process.

The recent detection of ethanolamine (EtA, HOCH₂CH₂NH₂), a key component of phospholipids, i.e. the building blocks of cell membranes, in the interstellar medium is in line with an exogenous origin of life-relevant molecules (Rivilla et al. 2021). However, the stability and survivability of EtA molecules under inter/circumstellar and Solar System conditions have yet to be demonstrated. Starting from the assumption that EtA mainly forms on interstellar ice grains, we have systematically exposed EtA, pure and mixed with amorphous water (H₂O) ice, to electron, ion, and thermal processing, representing ‘energetic’ mechanisms that are known to induce physico-chemical changes within the ice material under controlled laboratory conditions. Infrared (IR) and vacuum ultraviolet (VUV)

spectra of EtA-containing ices deposited and irradiated at 20 K with 1 keV electrons as well as IR spectra of H₂O:EtA mixed ice obtained after 1 MeV He⁺ ion irradiation have been collected at different doses. The measured column density of EtA underwent exponential decay upon electron and ion bombardment. The half-life doses for electron and He⁺ ion irradiation of pure EtA and H₂O:EtA mixed ice are derived to range between 10.8–26.3 eV/16u. Using the results in space conditions, we conclude that EtA mixed in H₂O ice is more stable than in pure form and it should survive throughout the star and planet formation process.

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Fragmentation of Complex Organic Molecules: Exploring the Pathways Leading to Prebiotic Precursors

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Abstract. Understanding the fragmentation of complex organic molecules under interstellar conditions is key to uncovering chemical pathways leading to prebiotic precursors. This study investigates the fragmentation of these molecules exposed to ionizing radiation, simulating conditions in the interstellar medium, particularly in photodissociation and protostellar regions. We focus on how photons and charge particles induce bond dissociation, generating reactive fragments that contribute to prebiotic chemistry. Specifically, ethanolamine was studied in both gas and ice phases, mimicking interstellar conditions. Our findings reveal the formation of prebiotic precursors such as CNH_4^+ and C_2NH_4^+ , as well as new functional groups in astrophysical ice analogues. These processes suggest pathways through which molecular fragments and modified ice surfaces could converge to produce prebiotic compounds, offering valuable insight into the chemical origins of life.

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