COST Action CA20129
“Multiscale Irradiation and Chemistry Driven Processes and Related Technologies”
(MultIChem)

Working Group 1 meeting

Hotel Örk
Hveragerði, Iceland
July 21-22, 2023

Booklet of Abstracts

Scope

The Working Group 1 meeting of the COST Action CA20129 "Multiscale Irradiation and Chemistry Driven Processes and Related Technologies" (MultIChem) will take place on **July 21-22, 2023** in Hveragerði, Iceland. The meeting is organized by MBN Research Center (Frankfurt am Main, Germany) and Carl von Ossietzky University of Oldenburg (Oldenburg, Germany).

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

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

Venue

The meeting will be hosted by Hotel Örk, Breiðumörk 1c, 810 Hveragerði, Iceland. The hotel is located in Hveragerði, one of Iceland's most popular destinations known as "The Hot Spring Town". The town known for its geothermal area with active hot springs is located in the south of Iceland, 45 km east (30 minutes) from the capital Reykjavík on Iceland's main ring road, Route 1.

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Program of the meeting

Friday, July 21

14^{15} – 14^{30}	**Meeting opening**
14^{30} – 16^{00}	**Session 1: Electron-, photon- and ion collisions with biomolecular systems (Chair: Thomas Schlathölter)** **Ilia Solov'yov**, Institute of Physics, Carl von Ossietzky University Oldenburg, Germany *Modelling photoinduced electron transfers in complex molecular systems* **Franck Lépine**, Institut Lumière Matière, Université Claude Bernard Lyon 1, Villeurbanne, France *First instants following XUV ionization in complex (bio-)molecules: towards attosecond experiments in proteins and DNA* **Hidetsugu Tsuchida**, Quantum Science and Engineering Center, Kyoto University, Japan *Damage process of nucleotide molecules in water by ion irradiation*
16^{00} – 16^{30}	Coffee break
16^{30} – 18^{00}	**Session 2: Collision, radiative and fragmentation processes (Chair: Himadri Chakraborty)**

	Thomas Schlathölter, Zernike Institute for Advanced Materials, University of Groningen, Groningen, The Netherlands *Implementation of a compact source for mass selected and conformationally pure biomolecular clusters* **Luca Gerhards**, Carl von Ossietzky University Oldenburg, Oldenburg, Germany *Modelling collision processes in complex molecular systems using VIKING* **Filipe Ferreira da Silva**, Universidade NOVA de Lisboa, Caparica, Portugal *Boron complexes stability under electron interactions*

Saturday, July 22

09^{30} – 11^{00}	**Session 3: Electron-, photon- and ion collisions with clusters and nanoparticles (Chair: Hannes Jónsson)** **Himadri Chakraborty**, Northwest Missouri State University, Maryville, USA *Femtosecond to attosecond electron dynamics in fullerene materials* **Jefferson Shinpaugh**, Department of Physics, East Carolina University, Greenville, USA *Nanostructured gold as a radiosensitizer for irradiation by ions* **Matthew Dickers**, School of Physics and Astronomy, University of Kent, Canterbury, UK *Atomistic modelling and structural characterisation of coated gold nanoparticles for biomedical applications*
11^{00} – 11^{30}	Coffee break
11^{30} – 13^{00}	**Session 4: Collision induced processes with organometallic molecules (Chair: Nigel Mason)** **Alexey Verkhovtsev**, MBN Research Center, Frankfurt am Main, Germany *Irradiation-induced fragmentation of organometallic complexes studied by means of reactive molecular dynamics* **Matija Zlatar**, Department of Chemistry, University of Belgrade, Belgrade, Serbia *Quantum chemical insight into excited states of organometallic molecules* **Oddur Ingólfsson**, Science Institute and Department of Chemistry, University of Iceland, Reykjavík, Iceland *Low energy electron induced fragmentation and formation of gold containing deposits from* $(CH_3)AuP(CH_3)_3$ *and* $[(CH_3)_2AuCl]_2$ *by focused electron beam induced deposition*
13^{00} – 14^{30}	Lunch
14^{30} – 16^{00}	**Session 5: Collision and radiation-induced chemistry processes (Chair: Matija Zlatar)** **Nigel Mason**, School of Physics and Astronomy, University of Kent, Canterbury, UK *Clusters, aerosols and microdroplets – Complex chemistry revealed* **Józef Sienkiewicz**, Gdansk University of Technology, Gdansk, Poland *Optimization of the femtosecond laser impulse for excitation and the spin-orbit mediated dissociation in the NaRb dimer* **Anatoli Popov**, Institute of Solid State Physics, University of Latvia, Riga, Latvia *Distinctive features of point defect annealing in irradiated ceramic materials*
16^{00} – 16^{10}	**Meeting closing**

Modelling photoinduced electron transfers in complex molecular systems

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Creatures as varied as mammals, fish, insects, reptiles, and migratory birds have an intriguing ‘sixth’ sense that allows them to navigate using the Earth's intrinsic magnetic field. A photoreceptor, cryptochrome, has been suggested to endow birds with magnetoreceptive abilities as the protein has been shown to exhibit the biophysical properties required for an animal magnetoreceptor to operate properly. Cryptochromes are flavoprotein photoreceptors originally identified in *Arabidopsis thaliana*, where they play key role in growth and development. Subsequently discovered in *prokaryotes*, *archaea*, and *eukaryotes*, cryptochromes were shown to be involved in the animal circadian rhythms. The unique biological function of cryptochromes arises due to the very special photoactivation reaction occurring in the proteins: exposure to blue light results in the reduction of flavin pigments that are bound by the cryptochromes, which leads to the formation of a spin-entangled pair of radicals, the so-called radical-pairs.

The mechanism by which night-migratory songbirds sense the direction of the Earth's magnetic field appears to possibly rely on the quantum spin dynamics of light-induced radical pairs in cryptochrome proteins located in the retina [1-4]. Cryptochrome binds internally the flavin cofactor (FAD), which governs it signaling through light-induced electron transfer involving a chain of four tryptophan residues, TrpA, TrpB, TrpC, TrpD. The recently demonstrated ability to express cryptochrome 4a from the night-migratory European robin (Erithacus rubecula), ErCry4a, and to replace each of the tryptophan residues by a redox-inactive phenylalanine, offers the prospect of exploring the roles of the four tryptophans [3].

However, despite decades of research, it is still unclear if cryptochrome is hosting the key radical pair needed for chemical magnetoreception, mainly because the molecular reactions of the radical pair in cryptochrome are not fully resolved yet. To advance the understanding of cryptochrome functioning, I will discuss the results of real-time QM/MM (quantum mechanical/molecular mechanical) electron transfer simulations based on the DFTB (Density Functional-based Tight Binding) approach. The results of these computations permit a comparison between simulation results and experimental measurements and provide a detailed microscopic insight into the sequential electron transfers along the tryptophan chain. Our results offer a route to the study of spin transport and dynamical spin correlations in flavoprotein radical pairs.

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First instants following XUV ionization in complex (bio-)molecules: Towards attosecond experiments in proteins and DNA

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High harmonic generation (HHG)-based light sources have had a major impact in photo-science as they combine the possibility to deliver high energy photons (VUV-XUV-soft X-ray), usually accessible at large scale facilities, with short pulse duration that allows to perform experiments with high time resolution (from picosecond to attosecond). In the past years, we have developed experiments where HHG sources allowed us to study ultrafast dynamics induced by the excitation of complex molecules by XUV radiation. In excited polycyclic aromatic hydrocarbons and diamontoid cations [1], [2] we observed how the deposited energy is spread in electronic [3] and vibrational degrees of freedom [4] on femtosecond timescale.

Here, we present results in which we study the quantum electron scattering of the photoionized electron on the molecular ion structure by measuring the scattering delay with attosecond precision. We show that information on the spatial hole distribution is imprinted in the measured delay. These experiments can be performed on model carbon based molecules as well as in biomolecules.

We have also shown that HHG-based time-resolved technics can be adapted to study molecular native ions as large as a protein, by combining ESI-MS-HHG technologies [5, 6, 7] providing information on the first steps following the ejection of an electron. These experiments demonstrate the possibility to perform experiments in complex biopolymers with attosecond precision and therefore pave the way to multiple time scale understanding of photoinduced processes in complex biomolecules.

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Damage process of nucleotide molecules in water by ion irradiation

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In the last few years, researchers have been studying the influence of liquid water on damage caused to biomolecules by radiation. This is because liquid water is a crucial component of biological substances. In this work, we studied how liquid water affects the damage nucleotides by ion beam irradiation. Our goal was to understand the damage process of biomolecules in the Bragg peak region of particle beam cancer therapy.

The experiments were performed using a 2 MV tandem-type Pelletron accelerator. The biogobical molecule used in this study was uridines 5'-monophosphate (UMP), which possesses a nucleotide structure. Two targets were used: a 0.226 mol/L UMP aqueous solution and a dry UMP target. The dry UMP target was formed by dropping UMP solution onto a Si substrate followed by natural drying. These targets were irradiated with carbon ion beams with energies ranging from 0.5 to 6.0 MeV. The emitted positive and negative secondary ions from the targets were measured using a time-of-flight mass spectrometer.

The mass spectrum for 4.0 MeV carbon ion irradiation is presented in Figure 1. The positive ion mass spectra showed that the decomposition ions from UMP were similar in the dry UMP target and the UMP aqueous solution. Hence, it is suggested that liquid water does not affect UMP dissociation processes. On the other hand, when examining the negative ion mass spectrum, it was observed that the decomposition ions produced from UMP varied depending on whether it was from a dry UMP target or a UMP aqueous solution. This indicates that there is a definite influence of liquid water. The influence implies that the reaction products of water caused by radiation may contribute to the damage of UMP in liquid water.

This talk will discuss how UMP damage yield and linear energy transfer (LET) are related. Scpecifucally, we look at how the decomposition ion yield is related to the electronic stopping power of UMP for dry UMP targets. We also analyze the relationship between decomposition ion yield and the electronic stopping power of water for aqueous UMP solutions.

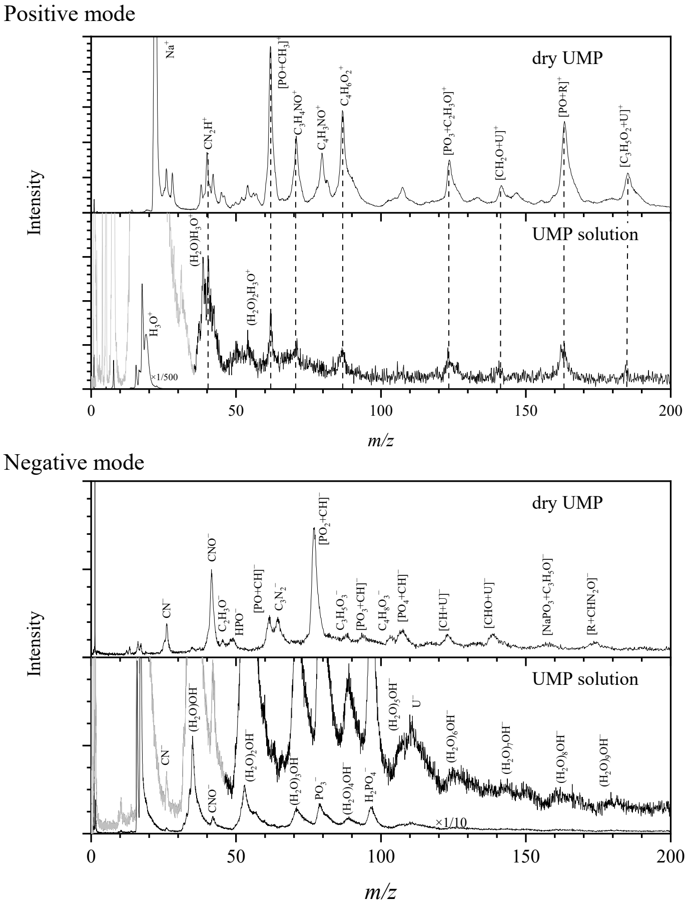

Figure 1: *The mass spectra of positively and negatively charged ions from dry UMP targets and UMP aqueous solutions, when exposed to a 4.0 MeV carbon ion beam, are displayed in panels (a) and (b), respectively.*

Implementation of a compact source for mass selected and conformationally pure biomolecular clusters

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For more than two decades, interactions of photons, electrons and ions with gas-phase biomolecules have been intensively studied to understand the molecular mechanisms of biological radiation damage. Early experiments focused on interactions with neutral nucleobases or amino acids, i.e. with single building blocks of biological macromolecules. These relatively simple systems can be brought into the gas phase by evaporation.

Biologically more relevant molecules, such as DNA strands, DNA-protein complexes or nanosolvated DNA are not sufficiently stable for evaporation. Electrospray ionization has become the most common technique, to prepare gas-phase targets consisting of complex biomolecular ions [1].

Over the last years, we have combined electrospray ionization with radiofrequency ion guiding and trapping, to prepare targets of trapped mass-selected gas-phase DNA ions for experiments with multiply charged carbon ions at Bragg-peak energies [2,3]. In complementary studies using synchrotron radiation, we have investigated soft X-ray induced hydrogen transfer in gas-phase DNA [4].

One of the most challenging issues in experimental studies involving complex biomolecular systems is the enormous conformational space. Even under cryogenic conditions, gas-phase biomolecular targets often contain several different conformers. This is very problematic for the interpretation of experimental data and in particular for comparison to theoretical studies.

A well-established approach to reach conformational separation of molecular ions are ion-mobility techniques, where a staticelectric field drives bunches of molecular ions through an inert gas. Drift velocities can be related to the geometric cross section which corresponds to the molecular conformation. Experimentally, the conventioanl ion-mobility approach is particularly problematic in situations where compact and flexible solutions are required, for instance for interfacing with synchrotron or heavy ion beamlines: Ion mobility drift regions are typically several meters long and require kV potentials.

We have implemented an alternative ion-mobility approach, based on radiofrequency ion guiding along pathways realized on printed circuit boards. This approach does not require large voltage gradients, as the ions are transported along their path by means of traveling waves. The electrode structures are implemented on printed circuit boards. Based on this principle, we have realized a compact apparatus that allows for production of intense beams of protonated and deprotonated biomolecular ions, that are m/q selected and conformationally pure. The entire system is very compact and can easily be interfaced with lasers, synchrotron beamlines and MeV ion beamlines. In this presentation, we will present the experimental technique and show results of first proof-of-principle experiments.

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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 their subsequent influence on molecular structures at larger time and length scales.

At the microscopic level, accurately modeling 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. VIKING [4] combines different theories and program 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 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 optimizations, 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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Boron complexes stability under electron interactions

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The organic synthesis community finds the chemical properties of boroxine highly captivating due to their potential in generating groundbreaking molecular structures. Boroxine's remarkable capacity to transition between various geometric configurations of its N-coordinated boron atoms serves as a valuable asset in enhancing the pharmacological characteristics of drug delivery systems. This adaptability enables the optimization of features like molecular recognition and targeted interactions with specific molecules, making boroxine an invaluable tool in this field. Indeed, boroxine cages have gained prominence as a class category of functional nanostructures employed in host-guest chemistry. Furthermore, the creation of a two-dimensional boroxine framework using Triphenylboroxine has revealed extraordinary electronic and morphological attributes, which hold potential for application in the development of novel electronic devices.

In this communication there will be presented two studies describing the reactions initiated by LEEs with triphenylboroxine (TPB) [1] and 2,4,6-tris(4-formylphenyl)boroxine (TFPB) [2]. These studies were supported by quantum chemical calculations performed by Lucas Cornetta, Instituto de Física Gleb Wataghin, Universidade Estadual de Campinas. The first study findings indicate that TPB exhibits a high level of stability and energy selectivity upon electron interaction, which may explain its usefulness in a variety of biomedical and pharmaceutical applications. The second study suggests that TFPB properties may combine the potential radiosensitizer effect of benzaldehyde with the stability of the boroxine ring. The conclusions of these experiments at molecular level may contribute to the development of novel medical strategies, namely in anticancer therapy, including chemo-radiotherapy protocols.

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Femtosecond to attosecond electron dynamics in fullerene materials

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Understanding the photoinduced “hot” electron relaxation dynamics in fullerene molecules is valuable in photovoltaics and photothermal therapy. The former benefits from slower relaxation times that increase the carrier collection efficiency, while the latter gains efficacy from quicker relaxation resulting in the lattice thermalization. On the other hand, the knowledge of photoelectron emission time delay at fullerene giant plasmon (GP) excitation energies can be beneficial for quantum plasmonics with applications in nanophotonics, photocatalysis and the design of controlled slow electron sources. Of course, both processes have deep fundamental research interests. With easy availability of C_{60} and advances in the synthesis of endohedral C_{60} in gas phase, in solution or as films [1], these materials render natural laboratories to probe ultrafast processes by ultrafast transient absorption spectroscopy (UTAS) or time-resolved photoelectron spectroscopy (TRPS).

In this computational study, the relaxation simulation is carried out by electron-phonon coupled non-adiabatic molecular dynamical workflow within a DFT framework [2]. While this method relies on an independent particle approach, a configuration-interaction singles description of the many-body effects produced similar results [2]. The photoemission time delay is computed *via* the Eisenbud-Wigner-Smith (EWS) track employing linear-response time-dependent DFT [3]. This method enabled collective many-body effects to couple with the emerging photoelectrons at the onset of the plasmon excitations.

In conclusion, therefore, these three orders of magnitude quickening of the dynamics from the relaxation to the ionization must be due to the coupling of electrons with the phonon (lattice vibration) in the former but with the plasmon (electron collective process) in the latter.

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Nanostructured gold as a radiosensitizer for irradiation by ions

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Nanostructured materials are widely being studied as radiosensitizers to increase the efficacy of radiation therapy in the treatment of cancer. While many such studies have been conducted for traditional high-energy photon radiation therapy, fewer studies exist for hadron therapy which is now rapidly expanding as a treatment modality. At East Carolina University, we are studying various materials, including nanostructured metals and metal oxides, to explore their properties as radiosensitizers for ion beam radiation. Our recent results for enhanced tumor cell killing are presented for *in-vitro* irradiation by protons of malignant prostate and breast epithelial cells treated with metallic nanoparticles in an energy range approaching the Bragg peak. The experiments were conducted in the ion beam facility at East Carolina University using the recently upgraded cell irradiation beamline.

In addition, we are expanding current Monte Carlo track structure simulation models to include swift-ion-induced secondary electron production from gold surfaces. Furthermore, to explore the difference between electron emission from the bulk and from nanostructured surfaces, we have measured doubly differential electron emission yields from gold surfaces (foils), hydrated gold surfaces, and from gold nanostructures induced by fast proton and carbon ion impact. Representative spectra for electron emission induced by 2-MeV proton impact on a gold foil and 10-nm gold nanoparticles will be shown, where enhanced low-energy electron emission is clearly observed. These data suggest the importance of the surface structure on low-energy electron emission, which may affect radiation damage from secondary electrons in the cellular environment and influence cell killing.

Atomistic modelling and structural characterisation of coated gold nanoparticles for biomedical applications

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We present the results of atomistic structural characterisation of 3.7 nm gold nanoparticles (NPs) coated with polymer polyethylene glycol (PEG)-based ligands of different lengths (containing 2-14 monomers) and solvated in water [1]. The system size and composition are selected in connection to several experimental studies of radiosensitisation mechanisms of gold NPs [2]. We characterise the coating structure and distribution of water close to the NP surface by means of molecular dynamics simulations using the MBN Explorer [3] software package. The results of simulations carried out in this study, combined with the results of our recent study [4], and those from the field of polymer physics, are used to calculate key structural parameters of the coatings of radiosensitising gold NPs. On this basis, connections between the coating structure and distribution of water are established for different NP sizes as well as lengths and surface densities of coating molecules. The quantitative analysis of water distribution in the vicinity of coated metal NPs can be used to evaluate the radiosensitising effectiveness of a particular NP system based on the proximity of water to the NP metal core, which should impact the production of hydroxyl radicals and reactive oxygen species in the vicinity of metal NPs exposed to ionising radiation [5,6].

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Session 4 “Collision induced processes with organometallic molecules”

Irradiation-induced fragmentation of organometallic complexes studied by means of reactive molecular dynamics

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Irradiation-induced fragmentation and chemical transformations of molecular systems play a key role in nanofabrication processes, particularly in focused electron beam-induced deposition (FEBID), where organometallic compounds break up due to the irradiation with focused particle beams [1,2]. An atomistic-level understanding of irradiation-driven chemistry processes (i.e., bond cleavage and further reactivity) of various molecular (including organometallic) systems can be achieved computationally by means of classical reactive molecular dynamics (RMD) [3] and irradiation-driven molecular dynamics (IDMD) [4] methodologies using the advanced software package MBN Explorer [5]. Developing such an understanding is at the core of several ongoing European research projects, such as the H2020 project “Irradiation driven nanofabrication: computational modelling versus experiment” (RADON) and the COST Action CA20129 “Multiscale irradiation and chemistry driven processes and related technologies” (MultIChem) [6].

This talk will report the results of the recent and ongoing RMD & IDMD studies of irradiation-induced fragmentation of several organometallic systems – iron pentacarbonyl, $Fe(CO)_5$, and trimethyl (methylcyclopentadienyl)platinum(IV) ($MeCpPtMe_3$), which are widely used precursors for the deposition of metal-containing nanostructures using FEBID [7].

Particular focus will be made on analyzing the effects of the molecular environment on the fragmentation of precursor molecules after their ionization. The role of the molecular environment has been analyzed by means of RMD simulations [8] by comparing the irradiation-induced fragmentation dynamics of an isolated $Fe(CO)_5^+$ ion with that of a $Fe(CO)_5^+$ ion embedded into an argon cluster. The simulation results [8] indicate strong suppression of the release of CO ligands of the $Fe(CO)_5^+$ ion embedded into an argon cluster, the effect observed experimentally in Ref. [9].

We will also briefly overview the latest RMD results of irradiation-induced fragmentation of a $MeCpPtMe_3$ molecule [10]. Recent electron-ionization mass-spectrometry experiments with $MeCpPtMe_3$ performed at the J. Heyrovský Institute of Physical Chemistry (Prague, Czech Republic) observed different fragment ions corresponding to a loss of one or several CH_3 ligands, and the appearance energies of these fragments were determined with high resolution [10]. We will present the first results of the RMD-based quantitative analysis of different ionic fragments and their appearance energies for the fragmentation of a single $MeCpPtMe_3$ ion in the gas phase.

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Quantum chemical insight into excited states of organometallic molecules

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

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

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Session 4 “Collision induced processes with organometallic molecules”

Low energy electron induced fragmentation and formation of gold containing deposits from $(CH_3)AuP(CH_3)_3$ and $[(CH_3)_2AuCl]_2$ by focused electron beam induced deposition

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Gold nanoparticles have found applications in a wide range of medical imaging, diagnostics, and therapy and several physical and chemical methods have been established for their fabrication. [1,2]. However, methods to fabricate well defined 3D, spatially ordered gold nanostructures are less advanced. Due to the optoelectronic properties of gold nanostructures such arrangements have high potential in plasmonics and in general in the sensor technology and methods to create these are thus called for. Focused electron beam induced deposition (FEBID) [3] is a promising approach – a single step nano-print method, ideally suited for fabrication of 3D free-standing nanostructures of as good as any shape on any surface topography.

In FEBID a precursor gas is introduced close to a substrate surface under high vacuum and the gas molecules that physisorbe on the surface are decomposed under a tightly focused high-energy electron beam. The volatile fragments are pumped away while the non-volatile build the deposit. Lateral control is achieved by moving the beam and vertical growth by variation of the dwell time. For metallic nanostructures, the precursor molecules are generally organometallics and in the ideal case, all ligands are cleaved of and pumped away, leaving a pure metal deposit. Currently, however, incomplete decomposition of the precursor molecules and thus ligand contamination in the deposits remains the main challenge in FEBID.

Consequently, significant effort has been made in the last decade to design precursor molecules that enable high purity deposits. This is not a simple task as inelastically scattered and secondary electrons, produced through interaction of the primary beam with the substrate and the forming deposits, play a significant role in the fragmentation process. Hence, the electrons responsible for the decomposition have a wide energy distribution and may cause dissociation by as different processes as dissociative electron attachment (DEA), dissociative ionization (DI), and neutral and dipolar dissociation through electron excitation (ND and DD, respectively). [4] It is thus important to understand the underlying processes and their extent, and how these influence the deposits, to eventually be able to design high performance precursors.

Here we take a step in this direction and study three different gold precursors with different ligand structures, i.e., $(CH_3)AuP(CH_3)_3$ and $[(CH_3)_2AuCl]_2$. DEA and DI of these precursors is studied in the gas phase under single collision conditions and the appearance energies are determined for individual channels. These are compared to quantum chemical threshold calculations for the m/z ratios observed to aid the assignment of ions and the neutral counterparts formed in these processes and FEBID depositions are made under UHV to explore how the elementary processes observed in the gas phase are reflected in the composition of the deposits.

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Clusters, aerosols and microdroplets – Complex chemistry revealed

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Clusters form an intermediate between discrete molecular systems and bulk materials (solids or liquids) demonstrating distinct physical and chemical properties due to opportunities for both inter- and intra-cluster reactions. Similarly, aerosols and microdroplets have novel spectroscopic and chemical properties. The role of clusters, aerosols and microdroplets in many diverse areas of science and technology (for example in atmospheric sciences and atmospheric plasma technologies) and have recently been suggested as playing a key role in the origins of life. Therefore, new experimental methods (including acoustic levitation [1]) coupled to multiscale modelling are being developed.

In this talk I will discuss the current state of our knowledge of physical and chemical properties of clusters, aerosols and microdroplets and the new experimental and modelling methodologies being developed. Several examples will be given of applications of such research and the scientific and industrial challenges that may be addressed by collaborative programmes.

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Optimization of the femtosecond laser impulse for excitation and the spin-orbit mediated dissociation in the NaRb dimer

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Quantum dynamics is a growing discipline at the interface of chemistry, physics and materials science. It allows studying the behaviour of objects in a way, that emphasizes the quantum nature of their evolution in time. Quantum dynamics simulations are an indispensable tool for investigating processes such as chemical reactions, field-molecule interactions and quantum computing. The particular emphasis is placed on investigating the photoinduced dynamics of breaking (dissociation) and creating (association) of the chemical bonds in the molecular systems.

Using quantum dynamical methods, we have already studied rotational predissociation in LiH [1], metastable states in KLi [2], and dissociation channels of Ag_2^+ [3]. Here, we study the dynamics of multiple coupled states under the influence of an arbitrary time-dependent external field to investigate the femtosecond laser-driven excitation and the spin-orbit mediated dissociation in the NaRb dimer. In this process, the dimer is excited from the ground triplet state $1^3\Sigma^+$ to the $1^3\Pi$ state using the femtosecond laser impulse and the spin-orbit coupling between the $1^3\Pi$ and $2^1\Sigma^+$ states results in the singlet-triplet transition. The laser impulse parameters are optimised to obtain maximum yield in electronic states correlating with the first excited atomic asymptote. We observe the detailed population statistics and power-law decay of these states. Finally, the analysis of the population oscillations allows us to determine the optimal time delay for dumping the molecule to its absolute ground state [4].

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Distinctive features of point defect annealing in irradiated ceramic materials

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The industrial progress of 21st century could greatly benefit from development and exploitation of fusion reactors producing environmentally clean friendly electrical energy. One of a key problem here is need in new advanced materials able to operate under extreme conditions (high temperatures and intensive neutron/gamma radiation).

In this report, I will provide a brief overview of both general information on the status of the problems and the most interesting results obtained within the two EUROfusion Enabling Research Projects – "***Advanced experimental and theoretical analysis of defect evolution and structural disordering in optical and dielectric materials for fusion applications (AETA)***" (2019-2020) and "***Investigation of defects and disorder in nonirradiated and irradiated Doped Diamond and Related Materials for fusion diagnostic applications (DDRM) – Theoretical and Experimental analysis***" (2021-2023).

In a series of joint works by Institute of Solid State Physics, University Latvia, University of Tartu, Estonia and Karlsruhe Institute of Technology KIT, radiation damage of some promising functional materials (MgF_2, Al_2O_3, $MgAl_2O_4$, SiO_2, $Y_3Al_5O_{12}$, diamond and few more) from the priority list of the EUROfusion consortium was studied under neutron, proton, heavy ion [1-6].

The optical and dielectric, vibrational and magnetic properties of numerous crystalline and ceramic materials were carefully studied. Based on this study, we developed new theoretical methods able to evaluate and predict some important properties of these materials as well as their radiation damage evolution under extreme reactor conditions.

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