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Invited Talk / 1

Effect of protonation states on charge transfer in solvated systems

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The interaction between a molecule and X-ray radiation leads to a formation of core excited/ionized state. Due to the instability of this state an array of processes can occur upon its decay, such as photon emission or Auger decay. The introduction of solvent can not only effect these processes, but also cause new ones, like charge transfer.
In charge transfer, the exited electron delocalizes from the virtual orbital and is distributed among the surrounding solvent molecules. In experiments, we can identify this process by observing either normal Auger decay or signal for X-ray emission under the ionization potential. Theoretical methods such as TD-DFT or CASSCF can provide additional information, such as the character of the excited states from both the orbital stadpoint and the delocalization perspective.
Charge transfer can occur in various systems. In our research we focused on two biologically relevant ones. The first was propylamine, a simple organic amine used as a proxy for other amines, in its neutral and protonated state. Auger spectra were measured at the DESY synchrotron (P04 beamline). Theoretical XAS (X-ray absorption spectra) were modeled for the 1s orbital of nitrogen atom using TD-DFT. There we saw that in both gas-phase and solvent, the excited states were diffused, which led to the observation of charge transfer for propylamine in water. Charge transfer was observable also for its protonated state. The shape of the spectrum itself changed, where in solvated propylamine, the intensity of these pre-edge peaks lowered drastically and in propylammonium they were also shifted to higher energies.
The second system was cystein, solvated at both pH 5 and 12. For this system, RIXS spectra were measured at SOLEIL and theoretical XAS spectra were again modeled using the TD-DFT method. Whereas for solvated propylamine all exctited states were charge-tranfer states, in cysteine the first few states, two at pH 5 and one at pH 12, were localized.

Invited Talk / 2

Low-Energy Electron Attachment to 1,2,3-Triazole and 4-Bromo-1-ethyl-1H-1,2,3-triazole: Study of Dissociative Electron Attachment

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The 1,2,3-triazole ring is an important heterocyclic structural motif in medicinal chemistry owing to its excellent chemical stability, synthetic accessibility, and diverse biological activities [1,2]. Triazole derivatives serve as valuable building blocks for the development of pharmaceuticals and functional materials, making it essential to understand their interaction with low-energy electrons, which play a significant role in radiation-induced chemical processes [1–3]. This work presents a comparative investigation of low-energy electron attachment to 1,2,3-triazole and 4-bromo-1-ethyl-1H-1,2,3-triazole in the gas phase. The experiments were performed using a crossed electron–molecular beam apparatus coupled with a quadrupole mass spectrometer, enabling the detection and identification of negative ion fragments formed via dissociative electron attachment (DEA). Electron attachment to 1,2,3-triazole predominantly results in dehydrogenation, yielding the corresponding dehydrogenated parent anion. In contrast, electron attachment to 4-bromo-1-ethyl-1H-1,2,3-triazole is dominated by bromide formation, producing fragment anions corresponding to the naturally occurring isotopes $^{79}Br^-$ and $^{81}Br^-$. The observed fragmentation patterns demonstrate the pronounced influence of bromine substitution on the electron-induced dissociation dynamics of the triazole framework. These findings provide new insights into the structure-dependent electron attachment behaviour of substituted triazoles and contribute to a better understanding of electron-driven processes relevant to radiation chemistry and biologically important heterocyclic molecules [3].

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Invited Talk / 3

Direct imaging of the metastable uracil dynamics using multi-mass detection

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Nucleobases are photostable biomolecules with complex relaxation dynamics on picosecond timescales [1], making them an ideal testbed for exploring ultrafast fragmentation dynamics with atomic-scale precision. We employ the versatile transportable endstation for controlled molecules (eCOMO) [2] to investigate isolated uracil molecules as well as size-selected hydrated clusters [3].

Using strong-field photodissociation combined with multi-mass velocity-map imaging (VMI), we directly detect a metastable fragmentation pathway of the uracil cation, $\mathrm{C_4H_4N_2O_2^+} \rightarrow \mathrm{C_3H_3NO^+}, (m/q = 69) + \mathrm{HNCO}$, with an estimated lifetime of 1.03 ± 0.15 μs. Furthermore, the combination of multi-mass VMI and time-resolved analysis enables us to resolve energy-dependent fragmentation dynamics by assigning kinetic energy distributions to different fragmentation times on the microsecond timescale.

Overall, we present a new experimental approach for the direct detection of weak metastable fragmentation dynamics using a Timepix3-based multi-mass imaging detector. This technique enables the observation of weak metastable fragmentation channels that are typically inaccessible with conventional gated VMI or mass spectrometry.

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Invited Talk / 4

Equivariant Variational Autoencoders for Efficient Sampling of Path-Integral Monte Carlo Configurations

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Path-integral methods, such as Path Integral Molecular Dynamics (PIMD) and Path Integral Monte Carlo (PIMC), are widely used to investigate the quantum-mechanical properties of systems with complex electronic structures. Despite their high accuracy, these methods require substantial computational resources and often suffer from slow convergence due to the high dimensionality of the sampled configuration space.

To overcome these limitations, we propose a generative neural network approach based on a Variational Autoencoder (VAE) to improve the efficiency of PIMC sampling. The VAE learns a low-dimensional latent representation of high-dimensional imaginary-time configurations while retaining the relevant statistical properties of the input PIMC data. By sampling from the latent space, we can generate new statistically representative PIMC configurations.

To preserve translational and rotational equivariance of the physical system, we incorporate E(n)-Equivariant Graph Convolutional Layers (EGCLs) into both the encoder and decoder architectures, together with additional neural network layers and activation functions.

A key advantage of the proposed approach is its ability to generate large numbers of samples in parallel. After training, independent latent vectors can be sampled from the learned underlying distribution and simultaneously decoded into batches of PIMC configurations, enabling efficient generation of statistically representative samples. This framework provides a promising approach to reduce the sampling overhead associated with conventional PIMC simulations.

Furthermore, we demonstrate that the generated configurations reproduce the structural and thermodynamic properties of reference PIMC simulations, highlighting the potential of equivariant generative models as efficient accelerators for quantum statistical simulations of systems with complex electronic structures. [1]

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Invited Talk / 5

Electron collisions with microhydrated clusters of 8-(trifluoromethyl)thioadenine

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Radiotherapy has been well known as the principal modality for oncology treatment. In order to improve the efficacy of radiotherapy, chemical radiosensitisers have been studied and employed 1. However, the underlying molecular mechanisms to sensitise the cancer cells to ionising radiation of radiosensitisers are not yet fully understood.
Irrespective of the nature of primary radiation, the most abundant secondary particles generated under radiation are electrons. Electron collision studies play a central role in establishing a better understanding of radiosensitiser' s behaviour. The experiments can be performed under different conditions of the target radiosensitiser molecules. In this work, we have experimentally investigated interactions of electrons with microhydrated clusters of 8-(trifluoromethyl)thioadenine –ASCF3 –a new potential purine-based radiosensitiser 2 via two mechanisms: electron ionisation and electron attachment.
Experiments were conducted in a recently constructed setup in our laboratory. The apparatus consists of a molecular cluster source and a Nier-type electron source incorporating an orthogonally reflectron time-of-flight mass spectrometer. Upon electron ionisation, fragmentation is essentially quenched by the presence of the surrounding water molecules, the most prominent fragment is associated with a cleavage of neutral CF3. This fragment also prevails in the case of electron attachment, wherein we observed its stabilisation with some attached water molecules.
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Invited Talk / 6

DNA Origami as an Alternative for Data Storage

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The presentation will introduce DNA nanotechnology and its recent DNA data storage applications within the NEO consortium (neodna.eu).
The Crystallographer Nadrian Seeman proved that DNA could be used as building material for assembled 2D and 3D frameworks thanks to its natural base-pairing recognition (Guanine–Cytosine and Adenine–Thymine) [1]. However, the design and synthesis of these systems required several tedious processes, including annealing and filtration, leading to errors.
Therefore, motivated by this, Paul Rothemund developed the DNA Origami technique. Allowing the assembly of any desired shape by folding a single plasmid strand, named "scaffold", with complementary short single strands, called "staples", mixed in a one-pot simple reaction [2].
DNA Origami can be used in multiple nanotechnology applications, such as data storage. The increasing volume of digital data has created a growing demand for sustainable, long-term, high-density data storage solutions [3]. Therefore, the search for alternatives has led to DNA-based storage. DNA Origami nanostructures (DON) can be used as "breadboard" or "nodes" for encoding digital data in a specific arrangement controlled with nanometric precision [4]. This opens new opportunities for next-generation data storage technologies.

Acknowledgment: This work was supported by the European Union via project number 101115317, NEO (neodna.eu).

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Invited Talk / 7

Electron-Induced Chemistry of Bromotriazole: From Isolated-Molecule Mechanisms to Exploration of Pure and Hydrated Clusters Using Genetic Algorithms

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Understanding electron-attachment processes in complex molecular clusters requires reliable sampling of low-energy structures. However, the number of possible isomers increases rapidly with cluster size, making systematic exploration of the potential energy surface a major computational challenge. We address this problem using an in-house framework that combines genetic-algorithm-based global optimization with graph-based structure clustering [1,2]. Incorporating structural classification directly into the evolutionary search preserves chemical diversity while eliminating redundant candidates, resulting in a more efficient exploration of the potential energy surface.

We demonstrate this framework for dry and hydrated clusters of 4-bromo-2H-1,2,3-triazole (BHT). Triazole rings are widely used in pharmaceuticals, pesticides, polymers, and coatings, yet their high stability makes controlled transformation and environmental degradation challenging. As a complementary molecular-level study, we first investigate electron attachment to isolated BHT. Direct C–Br bond cleavage associated with the σ^*(C–Br) resonance competes with bromine roaming, leading to fragmentation and ring opening, as demonstrated experimentally by fragment anions that require cleavage of the triazole ring [3].

For clusters of BHT, as well as microhydrated monomers and dimers of BHT, the genetic algorithm enables efficient identification of chemically distinct low-energy structures. The results show that intermolecular interactions stabilize the triazole ring and increase the electron affinity. For both BHT monomers and dimers, hydration suppresses bromide loss through efficient solvation of the bromide anion. Instead, as long as the molecule is hydrated, evaporation of a single water molecule is always favored over other channels, providing an effective mechanism for energy dissipation.

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Invited Talk / 8

2D Electron Energy Loss and Resonances in Phenyl Cyanide

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The smallest nitrile-substituted aromatic compound Phenyl cyanide (C_6H_5CN) has recently gained substantial attention since it has been detected in the interstellar medium (ISM). Under interstellar conditions, radiation-induced secondary electrons with kinetic energies in the tens of electronvolts [1] drive chemical pathways by forming temporary negative ions (resonances). These resonant states significantly enhance molecular vibrational excitation and bond-breaking processes. This work combines experimental and theoretical approaches to probe the temporary anion states of Phenyl cyanide, their role in vibrational excitation, and the mechanism of low-energy dissociative electron attachment (DEA).

Experiment: Electron-scattering measurements were conducted using a high-resolution (18 meV) electrostatic spectrometer featuring a hemispherical electron monochromator and analyzer at a fixed scattering angle of 135°. Two-dimensional electron energy loss spectroscopy (2D-EELS) [2] was utilized to map out specific and unspecific vibrational decay channels. DEA cross-sections yielding CN^- fragments were measured on a trochoidal time of flight setup and calibrated using a high-resolution setup.

Theory: Resonance positions, widths, and Dyson orbitals were computed at the neutral equilibrium geometry using complex absorbing potential extensions of equation-of-motion coupled-cluster theory (CAP-EOM-EA-CCSD/aug-cc-pVDZ+4s3p2d). Non-resonant EELS intensities were simulated using Born-approximation based integral cross-sections.

The CAP-EOM-EA-CCSD [3] calculations identified several π^* shape resonances. The positions of the higher-lying resonant states show excellent agreement with experimental features:

- 1^2B_1 (0.36 eV, $\Gamma = 0.03$ eV): A very narrow, dipole-stabilized resonance correlating with the bound valence anion ground state ($^2B_1$).
- 1^2A_2 (0.88 eV, $\Gamma = 0.02$ eV): A highly narrow state whose geometry relaxation (~ 0.18 eV) keeps it close to the valence ground state.
- higher states: Broad shape resonances computed at 1^2B_2 (2.23 eV / 2.69 eV), 1^2A_1 (2.46 eV), and 2^2B_1 (3.28 eV).

This work provides a comprehensive experimental and theoretical map of the resonant states in Phenyl cyanide. The results highlight the dual role of its large dipole moment (~ 4.5 D) in stabilizing narrow valence resonances and supporting a dipole-bound state that acts as an entrance channel for statistical vibrational excitation.

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Invited Talk / 9

Electron Attachment to 2-Bromo-5-Nitrothiazole and Nimorazole: Effects of Microhydration

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During radiotherapy, tumour tissue is irradiated with high-energy radiation with the goal to destroy as many tumour cells as possible while at the same time keeping the collateral effects on healthy tissue low. Nimorazole (Nimo) acts as an important example of a radiosensitizer, as it was shown to increase the survival rates of patients with supraglottic larynx and pharynx carcinoma, compared to patients receiving radiotherapy without nimorazole.[1] However, as the radiosensitizing properties could still be improved, other potential radiosensitizers are currently under investigation. One such example is 2-bromo-5-nitrothiazole (BNT). A crucial step of radiosensitization seems to be reduction of the radiosensitizer, e.g. through attachment of secondary electrons.
Therefore, in this contribution, we investigate the behaviour of BNT and Nimo upon attachment of low-energy electrons. To better understand the influence of the biological environment, we analyse the effects of microhydration. We furthermore investigate ionization of microhydrated BNT and Nimo to obtain a more complete image of how these molecules interact with electrons. Experimentally, the systems are studied using a crossed electron-molecular beam setup incorporating a time-of-flight mass spectrometer. The experimental findings are complemented with quantum chemical calculations, using a genetic algorithm[2] combined with graph-based structure clustering[3] to obtain molecular structures.

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Invited Talk / 10

Electron Induced Reactions in Formic Acid Clusters Doped with Sodium

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With experimental and theoretical approach combined, we investigated chemical reactions in formic acid (FA) clusters doped with sodium after low energy electron attachment. Clusters were created in supersonic expansion, and the anions were probed with a reflectron time-of-flight mass spectrometer. Calculations were preformed at the M062X/aug-cc-pvdz level of theory using Gaussian 16. Three main series containing sodium were present in the spectra - the strongest can be assigned to $[FA_n - 2H]^-$·Na, two other less pronounced are $[FA_n - H]^-$·Na, and $[FA_n]^-$·Na. Calculations were performed for all the three experimentally found series and also for neutral FA_n·Na. Theoretical results have shown that in neutral clusters a Na^+ $HCOO^-$ pair and a radical $HC(OH)_2$ are formed. The radical can further react after electron attachment and new molecules are formed by reduction of formic acid. Cluster structures and energetics of the above mentioned processes are discussed.

Poster / 1

Probing Radiosensitizers and Radioprotectors via DNA Origami-Based Platforms

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Understanding the molecular mechanisms of radiation-induced DNA damage across diverse environments is critical for advancing applications in cancer radiotherapy, nanodosimetry, DNA-templated lithography, and DNA-based archival data storage [1]. Strategically modulating the response of DNA to ionizing radiation (i.e., using radiomodulators) enables precise control and optimization of processes utilized in these fields.

Current methodologies for evaluating DNA radiosensitizers and radioprotectors generally operate at two extremes: the molecular scale (e.g., gas-phase electron scattering and mass spectrometry) or the cellular level (e.g., in vitro clonogenic assays). The intermediate, condensed-phase regime remains significantly less explored due to a lack of methodologies capable of observing localized DNA damage within complex, microenvironmental matrices [2]. Bridging this gap is crucial to elucidate the precise pathways of radiation damage, establish a quantitative link between fundamental gas-phase cross-sections and macroscopic biological outcomes, and optimize protocols for controlled DNA modification and long-term macromolecular preservation, as the applications demand.

Here, we present DNA origami-based platforms for evaluating the radiosensitizing and radioprotective effects of chemically modified nucleosides and small molecules. DNA origami nanoframes with a central aperture are used to support isolated DNA strands containing nucleoside analogues, including 8-bromoadenosine and 2′-deoxy-2′-fluorocytidine [3], as well as 5-methylcytidine within CpG islands [4]. Following irradiation with high-energy electrons (16 MeV) or carbon ions (95 MeV/u), DNA damage is quantified through in singulo detection of double-strand breaks using atomic force microscopy (AFM). Plain DNA origami nanostructures also enable the evaluation of radical scavengers, including cysteine and 2-((aminopropyl)amino)ethanethiol, by measuring through AFM, delayed DNA fragmentation following high-dose irradiation. An important advantage of this platform is its compatibility with established DNA analysis techniques, including gel electrophoresis [5], PCR-based (polymerase chain reaction) methods [3,4], and nanopore sequencing, enabling complementary assessment of radiation-induced damage. Together, these approaches provide a versatile framework for identifying next-generation radiosensitizers and radioprotectors.

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Poster / 2

Different experiments with clusters of Polycyclic aromatic hydrocarbons

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Polycyclic aromatic hydrocarbon (PAH) molecules can be found in atmospheric aerosols as a result of combustion processes. In addition, they are omnipresent in interstellar space, where they can also condense in icy grain mantles. Thus, these species play important role in atmospheric chemistry and astrochemistry, and investigation of PAH clusters and their complexes with other molecules can elucidate the processes involving PAHs in atmosphere and interstellar medium. The PAH molecules and complexes are also interesting from the fundamental point of view with respect to electron attachment. Benzene (Bz) and naphthalene (Np) have negative electron affinities and support only short-lived transient negative ion (TNI) resonances. However, solvation can stabilize TNI, e.g. $(Bz)_1(Np)_1^-$ complex [1] or $(Np)_2^-$ dimer anion [2]. In larger PAHs, an excess electron can delocalize, resulting in a positive EA. For anthracene (An) and pyrene(Py), EA = 0.54 eV and 0.41 eV, respectively. EA also depends on the molecular structure: An and phenanthrene (Ph) both consist of three benzene rings $C_{14}H_{10}$, but Ph is L-shaped with EA ≤ 0.025 eV [3].

We investigate clusters of PAHs –also doped with various other molecules –in CLUster Beam experiment CLUB in Prague [4,5] using mass spectrometry after electron ionization or photoionization, and also investigating negative cluster ions after slow electron attachment. Complementary experiments are performed with PAH clusters in positively and negatively charged helium nanodroplets in Innsbruck on TOFFY2. The experiments are interpreted by theoretical calculations of the groups E. Pluhařová in Prague and M. Ončák in Innsbruck. From these experiments and calculations, a complex picture arises about the PAH cluster structure, stability, dynamics and interactions with electrons and photons of different energies [6-11] which will be presented and discussed at the meeting.

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Poster / 3

Decomposition of azoles by low energy electrons

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This contribution provides an overview of our recent work on the reactivity of low-energy electrons with molecules containing an azole ring, from pilot studies with tetrazoles [1] to detailed exploration of complex roaming dynamics in triazoles [2]. Conclusions about the potential of low-energy electrons to induce molecular isomerization and decay of these highly stable molecules are drawn from experiments with isolated molecules, as well as from cluster studies that model realistic environmental conditions. Further insights into the reaction mechanisms are provided based on collaborative work with theory groups.

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Poster / 4

Bromine Position Controls the Electron-Induced Fragmentation Patterns in Microhydrated Ethyl-Triazoles

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Low-energy electrons (LEEs), produced during the interaction of ionizing radiation with matter, can induce molecular transformations through the formation and decay of transient negative ions (TNIs) [1]. Brominated triazoles are of interest in this context because they exhibit efficient electron attachment and a variety of competing decay pathways [2]. While electron attachment to isolated brominated triazoles has been investigated previously, less is known about the influence of a local solvent environment on these processes.

In the present work, we study low-energy electron attachment to microhydrated clusters of two positional isomers, 4-bromo-1-ethyl-1,2,3-triazole and 5-bromo-1-ethyl-1,2,3-triazole. Experiments were performed using the Complex Cluster Beam (CLUB) apparatus at the Heyrovsky Institute of CAS [3]. Hydrated clusters were generated in a supersonic expansion, and energy-resolved anion mass spectra were recorded in the 0–10 eV electron-energy range.

Electron attachment to the hydrated clusters reveals distinct isomer-dependent decay dynamics. In both positional isomers, the dominant products are parent hydrated cluster anions, $M(H_2O)_n^-$, reflecting efficient stabilization of transient negative ions by the surrounding water molecules. The principal difference lies in the fragmentation channels: one isomer retains a strong dehydrogenation pathway, yielding abundant $(M–H)^-$ ions, whereas this channel is absent for the other. These results demonstrate that microhydration stabilizes electron-attached states in both molecules, while the molecular structure determines whether hydrogen-loss fragmentation remains competitive.

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Poster / 5

The reactivity of heteroclusters of hydrogen peroxide and aromatic molecules with electrons of different energies

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Hydrogen peroxide (H_2O_2, HP) belongs to the class of reactive oxygen species and serves as an important reservoir of radical species due to its relatively weak O–O bond. In biological environments, leakage of electrons from the electron transport chain may induce dissociative electron attachment to H_2O_2, leading to the formation of hydroxide anions (OH^-). Both OH radicals and OH^- are highly reactive and are widely investigated because of their role in oxidative damage processes in biological systems. The physicochemical properties of H_2O_2 are closely related to those of water, particularly due to its ability to participate in hydrogen-bond networks and compete with water molecules in interactions with DNA bases and other biomolecular sites.
Molecular clusters represent finite-size models of solvation environments and provide a useful approach for studying the influence of specific bonding motifs on molecular stability and intermolecular reactivity.
We investigated electron-induced reactions in large benzene, Bz, and naphthalene, Np, clusters containing adsorbed hydrogen peroxide molecules. Mixed neutral clusters, BznHPk and NpnHPk were formed via sticking collisions of clusters in molecular beams and H2O2 gas. They were subsequently exposed to electrons of different energy to investigate the fragmentation mechanisms and formation of negative ions after electron attachment. The resulting clusters ions were analyzed by time-of-flight mass spectrometry.
For benzene-based systems, the dominant ion series corresponded to peroxide-containing cluster anions of the type Bzn(H2O2)k- with up to five peroxide molecules attached, accompanied by oxygen-containing ions assigned as Bzn(H2O2)kO-.
In naphthalene clusters, additional oxygen-rich species, Npn(H2O2)kO2-, were observed together with pure naphthalene cluster anions, consistent with the positive electron affinity of larger naphthalene aggregates. Compared to benzene clusters, fewer peroxide molecules were stabilized in the naphthalene system.
The observed ion distributions indicate competing pathways involving stabilization of intact peroxide-containing negative complexes and electron-induced dissociation of H_2O_2 followed by secondary intracluster radical reactions. Due to the identical masses of H_2O_2 and H_2O + O combinations, the present measurements do not allow unambiguous distinction between intact peroxide adducts and rearranged oxygen-containing products. Nevertheless, the enhanced formation of O- and O_2-containing ions in naphthalene clusters suggests more efficient secondary electron-driven chemistry in these systems.

Poster / 6

"Magic" of hydrated polycyclic aromatic hydrocarbon clusters

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Hydrated clusters of four simple PAHs –naphthalene, cyanonaphthalene, anthracene, and phenanthrene –were investigated. The clusters were produced in a supersonic expansion, ionized by electron impact, and the resulting ions were analyzed by a reflectron time-of-flight mass spectrometer. The mass spectra reveal a pronounced enhancement of the signal intensities for the cluster ions $[(\mathrm{PAH})_m(\mathrm{H_2O})_4]^{+/-}$ and $[(\mathrm{PAH})_m(\mathrm{H_2O})_8]^{+/-}$. We further discuss these findings, present the experimental setup in detail, demonstrate how the experimental conditions influence the observed mass spectra, and complement the experimental results with theoretical calculations.

Poster / 7

Hybrid microsystems assembled by DNA origami scaffolds

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The integration of DNA origami with microscale objects provides a powerful route for creating hybrid colloidal architectures with programmable geometry and multifunctionality complexity. However, achieving precise bottom-up assembly of micron-sized particles remains a major challenge. Here, we present a fully bottom-up strategy for fabricating Janus-type optomechanical probes by interlinking polystyrene and magnetic microspheres using a 24-helix bundle (24HB) DNA origami nanostructure as a selective and functional scaffold. Leveraging the addressability of DNA origami structures, we design and chemically modify specific sequences at the left and right termini to conjugate streptavidin-coated polystyrene and azide-coated magnetic microspheres via biotin-streptavidin interactions and click chemistry, respectively. Additionally, the 24HB scaffold acts as a multifunctional platform for the spatially defined incorporation of fluorophores, quantum dots, and gold nanoparticles, demonstrating binding specificity and functional addressability. Structural integrity and selective DNA-mediated coupling are confirmed by fluorescence microscopy and transmission electron microscopy, which reveal localization of 24HB interlinks bridging the two microspheres [1]. We further demonstrate that the synthesized heterodimers exhibit robust mechanical stability under optical trapping. Using a single-beam optical tweezer, we show stable 2D and 3D confinement as well as orientation-dependent behavior arising from the intrinsic shape and material asymmetry of the janus-type probes. These findings establish DNA-origami-mediated assembly as a versatile platform for programming functions into hybrid microscale probes, with potential applications in optomechanics, sensing, targeted transport, and next-generations photonic and quantum technologies.

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Keywords: Hybrid Complex, DNA Origami, Optical Tweezers

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Poster / 8

ESPECDAS: Automating Multireference Calculations to Build a Database of Electronic Spectra for Identifying Potential DIB Candidates

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The search for molecular carriers of diffuse interstellar bands (DIBs) remains one of the longest-standing open problems in astrophysics. While C_{60}^+ is the only DIB carrier firmly identified so far 1, modern high-resolution observations suggest that small molecules, including diatomics, may contribute to some DIB systems [2]. However, accurate experimental or theoretical gas-phase reference spectra are not yet available for many candidates. A systematic computational database could therefore guide targeted laboratory and astronomical studies toward the most interesting regions of the chemical search space and, more generally, substantially accelerate the assignment of astrophysical signals.

Generating such a database requires reliable electronic spectra for large numbers of molecules. Multireference methods are ideally suited to this task, but they are not applicable as black-box methods. For an individual molecule, electronic states and active spaces are typically selected manually on a case-by-case basis. In large-scale systematic studies, however, these choices become a major bottleneck. This leads to a central methodological question: can multireference electronic spectra calculations be automated sufficiently to generate reliable reference data at scale?

Here, we present the *Electronic Spectroscopy Database for Astrochemical Studies* (ESPECDAS), an automated workflow and database ecosystem for calculating electronic spectra of astrochemically relevant diatomic molecules. The electronic structure workflow is designed to cover excitation energies of up to approximately 7 eV. Molecular states are generated from atomic terms using Wigner–Witmer rules and tabulated atomic energy levels. AVAS-CASCI scans are used to construct and refine active spaces and to select relevant groups of states. State-averaged CASSCF calculations provide reference functions for subsequent state-specific X2C-MRCI+Q calculations [3]. Orbital occupations, transition-dipole continuity, avoided crossings, curve smoothness, and state degeneracies are monitored to assess state character and potential-energy-curve quality. The resulting simulated rovibronically resolved electronic spectra are collected in a database and made accessible through a web application and Python API, enabling searches based on characteristic rovibronic spectral patterns [4].

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Poster / 9

Advancement of FLASH effect for cancer therapy: Exploring the elementary processes of radiation chemistry induced at ultra-high dose rate conditions

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We aim to investigate the FLASH effect in well-defined solutions of bioactive molecules using short-pulse X-ray free-electron laser (XFEL) radiation. Radiotherapy operating at ultra-high-dose rates (UHDR, > 40 Gy/s) and short irradiation times (< 500 ms) shows preserved tumor-control efficacy with markedly reduced toxicity towards normal tissues, a phenomenon referred to as the FLASH effect [1]. Despite its rapid emergence as a transformative concept in radiation sciences, the mechanisms of the FLASH effect and their connectivity across radiolytic stages remain poorly understood [2,3]. One reason is limited access to ionizing radiation sources capable of delivering the required UHDR.
The XFEL radiation at the European XFEL facility, with its high brilliance, enables reaching ultra-high dose rates over TGy/s and thus may allow the investigation of energy deposition, transient radical formation, and other ultrafast phenomena occurring in physical, physico-chemical, and chemical phases that cannot be probed elsewhere. A core component of this project is the development of validated fluorescence and super-Fricke dosimetry tailored to UHDR conditions, supported by the design of pressure-resistant, chemically inert cuvettes compatible with XFEL safety and operational constraints. The present study is designed for the future realization of the experiment with an unfocused beam to reach homogeneous dose deposition in liquid samples. For irradiation, a broad band of UHDR will be applied to investigate occurring radiation-chemical and molecular processes and thus elucidate fundamental mechanisms of the FLASH effect.
By clarifying the fundamental physics and chemistry underlying the FLASH effect, these outcomes will provide insights that may facilitate the implementation of FLASH radiotherapy into practice with improved safety and reduced tissue toxicity. The present study will thereby enable the development of a future full beamtime proposal at the European XFEL facility.

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Poster / 10

Parallel Transport Diabatization using Neural ODEs

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Understanding non-adiabatic processes is essential for describing many chemical and physical phenomena, particularly in transition-metal complexes and photocatalysis. Their simulation requires potential energy surfaces and electronic couplings, but direct electronic-structure calculations are computationally demanding. Moreover, adiabatic potential energy surfaces become non-smooth near conical intersections, making them difficult to fit and use in long-time dynamics simulations.
Diabatic representations provide smooth potential energy surfaces, with electronic couplings appearing as off-diagonal elements of a potential energy matrix. However, constructing such representations remains challenging because of the gauge freedom of the electronic states and the topological effects associated with conical intersections.
We present a fully differentiable diabatization approach based on parallel transport using Neural ODEs. The method combines a limited set of non-adiabatic coupling data with a larger set of adiabatic energies to construct smooth diabatic potential energy surfaces. We demonstrate accurate results, correct Berry-phase behaviour, and applications to LiF and NO_2.

Poster / 11

Low-Energy Electron Attachment to 4-Bromo-2H-1,2,3-Triazole: Dissociation Dynamics

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Triazoles and their derivatives are widely used structural units in chemistry and pharmaceuticals that are valued in click chemistry for their high stability. However, the addition of lowenergy electrons can lead to significant molecular fragmentation and rearrangement, thereby opening potential pathways for "retro-click" reactions [1]. In this work, we investigated the electron-induced dynamics of 4-bromo-2H-1,2,3-triazole using molecular dynamics (MD) simulations. The trajectories were calculated using the ABIN software package, which was coupled to Gaussian 16 for all quantum chemical calculations at the BLYP/6-31+G(d) level of theory. The dynamics were evaluated for incident electron energies ranging from 0.0 to 0.6 eV, depositing a total internal excess energy of 1.6 to 2.2 eV into the transient negative ion relative to the optimized ground state of the neutral molecule. To systematically classify the complex reaction channels and structural variations, a graph-based structure clustering approach was applied [2].

Across all 73 analyzed trajectories, the primary step following electron attachment is C–Br bond dissociation, occurring with a yield of 100 %. This happens fast, starting as early as 84 fs, with a typical dissociation timescale between 100 and 130 fs. Furthermore, we observed Br-atom roaming and reattachment to the triazole ring in over 30 % of the cases. On the picosecond timescale, intra-molecular energy redistribution drives secondary fragmentation. Here, the bond dissociation between the second and third nitrogen atoms occurs, leading to ring opening in approximately 23 % of the cases.

Overall, these simulations provide detailed insights into how primary C-Br dissociation competes with bromine roaming and delayed ring opening during electron attachment to 4-bromo-2H-1,2,3-triazole.

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