11th International Meeting on Atomic and Molecular Physics and Chemistry

# IMAMPC 2022

# BOOK OF ABSTRACTS

Villa Lanna, Prague, June 13-17, 2022

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# 11th International Meeting on Atomic and Molecular Physics and Chemistry

June 13-17, 2022
Villa Lanna, Prague, Czech Republic

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|  | Monday | Tuesday |  | Wednesday |  | Thursday |  | Friday |  |
|---|---|---|---|---|---|---|---|---|---|
| 08:45 |  | **Opening** |  |  |  |  |  |  | 08:45 |
| 09:00 |  | **Merkt** *Precision measurements of the dissociation energy of molecular hydrogen* |  | **Ye** *Quantum gas of polar molecules* |  | …recovering… |  | **Departures** | 09:00 |
| 09:15 |  |  | **Shagam** |  | **Maclot** |  | **Choi** |  | 09:15 |
| 09:30 |  |  |  |  |  |  |  |  | 09:30 |
| 09:45 |  | **Paul** *Mutual neutralization in sub-eV $C_{60}^{+}+C_{60}^{-}$ collisions* |  | **Koza** *Towards collisional cooling of polyatomic molecules* |  |  |  |  | 09:45 |
| 10:00 |  | **Piekarski** *Benchmarking of triazole binders* |  | **Shagam** *Trapped chiral molecular ions for probing weak force parity violation* |  | **Kumar** *Bound electron enhanced radiosensitisation of nimorazole upon charge transfer* |  |  | 10:00 |
| 10:15 |  |  |  |  |  | **Kierspel** *MS SPIDOC: mass spectrometry meets single particle imaging* |  |  | 10:15 |
| 10:30 |  | **Lehman** *Mid-infrared frequency comb spectroscopy for chemical reaction kinetics* |  | **Lushchikova** *Chemistry and physics in multiply charged helium nanodroplets* |  | **Bull** *Ultrafast dynamics of isomer-selected molecules* |  |  | 10:30 |
| 11:00 |  | **Coffee Break** |  | **Coffee Break** |  | **Coffee Break** |  |  | 11:00 |
| 11:30 |  | **Hofierka** *Many-body theory of positron binding in polyatomic molecules* | **Lehman** | **Bischoff** *Quantitative study of enantiomer-specific state transfer* | **Mašín** | **Veselinova** *Accurate global $^{3}A''$ potential energy surface for the $O+C_2(^{1}\Sigma_g^{+}, ^{1}\Pi_u)$ reaction* | **Rohdenburg** |  | 11:30 |
| 11:45 |  | **Klimešová** *Ion dynamics in laser-irradiated helium gas around a nanoparticle* |  | **Khan** *Recent results on the ion-molecule reactive scattering* |  | **Badin** *Theoretical study of ion-ion collision in iodine plasma for spacecraft propulsion* |  |  | 11:45 |
| 12:00 |  | **Ezra** *Ab initio quantum analysis of the strong field dissociation process - angular momentum analysis* |  | **Huo** *The changes in electronic structure of PAH cations induced by hydrogenation* |  | **Rademacher** *Electronic spectroscopy of $H_2O@C_{60}^{+}$ and $D_2O@C_{60}^{+}$* |  |  | 12:00 |
| 12:15 |  | **Lengyel** *Size effects of tantalum cluster cations on simultaneous activation of methane and carbon dioxide* |  | **Tomza** *Quantum control of ultracold ion-atom collisions* |  | **Arismendi** *Data-driven approaches for modelling non-aqueous electrolytes* |  |  | 12:15 |
| 12:45 | **Registration Start** | **Barreiro Lage** *Non-trivial fragmentation on photoionized Diketopiperazines: new insights on prebiotic chemistry* |  | **Onvlee** *Unravelling controlled chemical reactions* |  | **Chiarinelli** *Insights in the structure of homogeneous and hydrated uracil clusters* |  |  | 12:45 |
| 13:15 | **LAB Afternoon** | **Lunch** |  | **Lunch** |  | **Lunch** |  |  | 13:15 |
| 14:30 |  | **González** *A theoretical journey from DNA building blocks to bioreceptors* | **Ončák** | **Free Afternoon** |  | **Wales** *Energy landscapes: from molecules and nanodevices to machine learning* | **Martinez** |  | 14:30 |
| 15:15 |  | **Rohdenburg** *Nanofabrication with layers of mass-selected ions* |  |  |  | **Šulc** *DNA nanotechnology: from coarse-grained modeling to experimental realization* |  |  | 15:15 |
| 15:45 |  | **Anstöter** *Using theory to pull back the curtain on experiment* |  |  |  | **Mašín** *Molecular photoionization in the weak- and strong-field regimes studied by the ab initio R-matrix method* |  |  | 15:45 |
| 16:15 |  | **Maclot** *Diamond(doid)s are a physicist's best friend* |  |  |  | **Noble** *Studying the competition between anionic and neutral excited state pathways in aromatic anions.* |  |  | 16:15 |
| 16:45 |  | **Coffee Break** |  |  |  | **Coffee Break** |  |  | 16:45 |
| 17:15 |  | **Chatterjee** *Histidine tautomerism modulated misfolding mechanism of prion protein: new insights from replica exchange molecular dynamics* | **Lushchikova** |  |  | **Best Hot Topic Award** | **Sanz-Sanz** |  | 17:15 |
| 17:30 |  | **Yan** *Uptake of organic molecules on hydrated HNO3 clusters: The effect of molecular properties on uptake cross sections* |  |  |  | **Dutta** *Light matter interactions in DNA origami assembled plasmonic nanostructures for single molecule spectroscopic study* |  |  | 17:30 |
| 17:45 |  | **Montes de Oca** *Ab initio characterization of noble gas containing molecules with astrochemical interest: data-driven intermolecular potential and spectroscopic data* |  |  |  |  |  |  | 17:45 |
| 18:00 |  | **Schewe** *Investigating the electrolyte-to-metal transition in liquid alkali-metal ammonia solutions* |  |  |  | **Martinez** *Light-driven reactions in DNA* |  |  | 18:00 |
| 18:30 |  | **Ončák** *Hydrated metal ions: nanolaboratories for modelling of elementary (photo)chemical processes* |  |  |  | **Gatchell** *The stability of defective PAH and fullerene ions over long timescales* |  |  | 18:30 |
| 19:00 | **Welcome Reception** | **Poster Session & Refreshments** |  | **Conference Dinner at umedvidku.cz & beer bottling & Best Poster Award** |  |  |  |  | 19:00 |

# Contents

# Precision measurements of the dissociation energy of molecular hydrogen

Fédéric Merkt

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Few-electron atoms and molecules are attractive systems for precision spectroscopy because their properties can be calculated with high accuracy by quantum-chemical methods.[1-5] The measurements serve to test theoretical predictions, ideally at the level where their accuracy is limited by the uncertainties of the fundamental constants or by unrecognized physical effects. I will report on precision measurements of energy intervals in cold samples of He, $H_2$ and $He_2$. In particular, we determine their ionization energies with a precision ($\Delta\nu/\nu$) better than $10^{-10}$ from high-resolution Rydberg spectra,[6-9] approaching the level where uncertainties in the size of the nuclei and the nuclear-to-electron mass ratios would limit the accuracy of otherwise exact calculations and calibration requires the use of primary frequency standards. Comparison will be made to recent theoretical results in the context of more-than-100-year- long experimental and theoretical efforts invested in the accurate determination of the properties of fundamental few-electron atoms and molecules. The primary focus will be on the dissociation energy of molecular hydrogen ($H_2$, HD and $D_2$)

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# Mutual neutralization in sub-eV $C_{60}^{+} + C_{60}^{-}$ collisions

Paul R.[1], Gatchell M.[1], Ji M.C.[1], Rosén S.[1], Larson Å., Björkhage M.[1], Schmidt H.T.[1], Cederquist H.[1], Zettergren H.[1]

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The detection of fullerenes in neutral and ionic forms in several extra-terrestrial environments [1][2][3] has been subsequently followed by extensive research, inquiring about the factors that constitute the molecule's formation and survival in these environments [4]. To advance the understanding of charge transfer processes involving fullerene molecules and their importance in e.g. space, we have performed mutual neutralization studies using the cryogenic storage ring facility, DESIREE [5]. With DESIREE, we are able to study sub-eV collisions between $C_{60}{}^{+}$ and $C_{60}{}^{-}$ ion beams, which marks the first-ever reported studies in this regime for molecular collisions. We detect neutral products formed in the process, that have an energy distribution with identifiable electronic excited states. The process is then modelled with the multi-state Landau-Zener method [6], using relevant interaction potentials [7][8] and coupling elements [9]. The excited states of $C_{60}$ used in the model were computed using Time Dependent-Density Functional Theory at the PBE0/6- 311++G(d,p) level of theory. The Landau Zener model predicts the total charge transfer cross section to be 5.52 x $10^{-11}$ $cm^2$, for a center-of-mass collision energy of 0 meV. This is a factor of 4-5 larger than for $H^+ + H^-$ collisions at the same collision energy [10]. The branching ratios subsequently obtained from the theoretical calculations follow the experimental trend observed for the same.sss

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# Benchmarking of triazole binders

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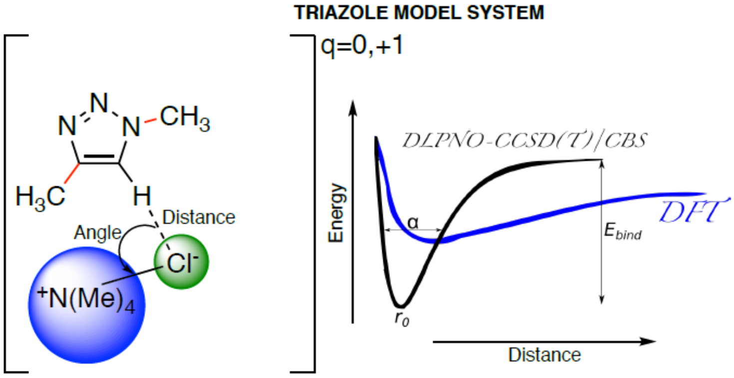

1,2,3-triazoles brought a lot of attention in organic chemistry, biology and medicine due to its reliable formation via click chemistry, which has become their "gold standard" synthetic route [1]. These molecules have unique bioisostere properties to be a building blocks as receptors in human bodies, in nature and also in the catalytic applications [2]. We focus on triazoles that play a key role in therecognition process using either the weak C-H type hydrogen bonds (HBs) or halogen bonds (XBs) and therefore being able to induce the transfer of the chiral information to the product via organocatalytic enantioselective reaction [3].

We have elucidated the accuracy of binding and redox properties of a set of 55 density functional (DF) approximations, including recently developed r2SCAN-3c meta-generalized gradient scheme. The characteristics focuses on a vastly used in catalysis triazole based model system [4] to be used as a key molecular fingerprint in the development of photo-activated anion binding catalysts. The assessment considers the fundamentally important in anion binding catalysis three body interaction; hydrogen bonding between triazole unit and chloride atom of the tertmethylammonium salt and is entrenched on comparing the potential energy curves calculated with DF theory and using "gold standard" domain-based local pair natural orbital version of the coupled-cluster theory with full singles and doubles and perturbative triples approach (DLPNO-CCSD(T)) and the complete basis set limit (CBS) extrapolated with focal point two point extrapolation basis sets (def2-TZVPP/def2- QZVPP). The choice of recently applied M06-2X/6-31G(d,p) level of theory with counterpoise correction giving excellent agreement with H-NMR experiments to determine the organoreceptor anion binding properties was justified. Finally, the most accurate DFs of a given rung were benchmarked for the reverse “click-triazole reaction” using molecular dynamics simulations against MP2 level.

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# Mid-infrared frequency comb spectroscopy for chemical reaction kinetics

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The 2005 Nobel Prize in Physics was awarded in part to John Hall and Theodor Hänsch for their development of optical frequency combs. As a simultaneously spectrally broadband and high resolution light source, frequency comb lasers have been successfully implemented in a variety of scientific fields ranging from metrology to high resolution spectroscopy. In this talk, I will highlight advances in trace gas detection using infrared frequency comb laser spectroscopy, with a focus on frequency comb use in chemical reaction kinetics and high resolution spectroscopy. I will give you an overview of frequency comb lasers, the design and implementation of a frequency comb spectrometer, and results from our newly built system. I will focus on our experimental results on the infrared spectroscopy of diiodomethane, $CH_2I_2$, its photodissociation and subsequent reaction.

# Many-body theory of positron binding in polyatomic molecules

Hofierka J.[1], Cunningham B.[1], Rawlins C. M.[1], Patterson C. H.[2], Green D. G.[1]

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Positrons bind to molecules leading to vibrational excitation and spectacularly enhanced annihilation (see [1] for a review). Whilst positron binding energies have been measured via resonant annihilation spectra for around 75 molecules in the past two decades [1], an accurate *ab initio* theoretical description has remained elusive. Of the molecules studied experimentally, calculations exist for only 6, and for these, standard quantum chemistry approaches have proved severely deficient, agreeing with experiment to at best 25 % accuracy for polar molecules, and failing to predict binding in non-polar molecules. The theoretical difficulty lies in the need to accurately account for strong positron-molecule correlations including polarisation of the electron cloud, screening of the positron-molecule Coulomb interaction by molecular electrons, and the unique process of virtual-positronium formation (where a molecular electron temporarily tunnels to the positron). Their roles in positron-molecule binding have yet to be elucidated.

We have developed a diagrammatic many-body description of positron-molecule binding in polyatomic molecules that takes ab initio account of the correlations [2]. We solve the Dyson equation for the positron quasiparticle wavefunction in a Gaussian basis, constructing the positron-molecule self-energy including the GW contribution that describes polarisation, screening and electron-hole interaction interactions (at RPA/TDHF/BSE levels), the ladder series of positron-electron interactions that describes virtual positronium formation, and the ladder series of positron-hole interactions. We have used it to calculate binding energies for a range of polar and non-polar molecules, focussing chiefly on the molecules for which both theory and experiment exist [2]. Delineating the effects of the correlations, we show, in particular, that virtual-positronium formation significantly enhances binding in organic polar molecules, and moreover, that it is essential to support binding in non-polar molecules including $CS_2$, $CSe_2$ and benzene. Overall, we find the best agreement with experiment to date (to within a few percent in cases). The method also enables the calculation of the positron bound wavefunction and of the positron-electron contact density (annihilation rate in the bound state).

Our approach can be extended to *ab initio* calculations of positron scattering and annihilation gamma spectra in molecules (currently underway), providing insight that should support the development of fundamental experiments and the myriad of antimatter-based technologies and applications. Moreover, the positron-molecule problem provides a testbed for the development of methods to tackle the quantum many-body problem, for which our results can serve as benchmarks.

This work is funded by DGG’s European Research Council grant 804383 “ANTI-ATOM”.

**References:**

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# Uptake of organic molecules on hydrated $HNO_3$ clusters: The effect of molecular properties on uptake cross sections

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Aerosol particles containing organic matter make up a significant proportion of the atmosphere, influencing global climate directly by interacting with solar radiation or by affecting cloud properties. The vast majority of such particles are produced by nucleation from vapor in a process known as gas-to-particle conversion. Through joint experimental and computational studies, we investigate the uptake of organic molecules on pre-existing hydrated $HNO_3$ particles. In our experiment, the $HNO_3/H_2O$ particles pass through a chamber filled with a particular gas, the molecules collide with the particles and can stick to the surface. The efficiency of this process is given by the uptake cross section, determined by mass spectrometry [1,2]. Our primary goal is to identify the specific requirements of a given neutral organic molecule to be efficiently captured by acid particles. Therefore, we measure the uptake cross section of molecules with different functional groups, such as alcohols, carbonyls, and carboxylic acids, or reveal the effect of double bonds on uptake efficiency. Further, we compared isomers of butanol to examine steric effects, as well as C1-C5 alkyl alcohols to analyze hydrophobicity on uptake cross sections. Lastly, simulations of the experiment are performed using a computational approach currently under development, which combines Born-Oppenheimer molecular dynamics and the semiempirical electronic structure method, to estimate the uptake cross sections and probabilities and compare them to the experimental results.

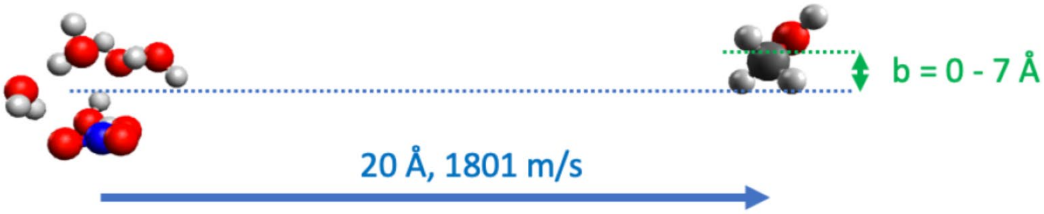

Figure illustrating the approach used for the determination of the uptake cross section and probability.

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# Ab initio quantum analysis of the strong field dissociation process - angular momentum analysis

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Simulating photo-dissociation processes from first principles is a challenging task. The difficulty is due to the vast Hilbert space dimension that is required for a full quantum description. Coupling the external electromagnetic field and the transition dipole moment induces transitions between electronic states. Each electronic transition is accompanied by an angular momentum change of one unit of $\hbar$. Thus, the dissociation process achieved by a strong field leads to a significant change in the angular momentum. Therefore, the exact calculation has to include all angular momentum quantum states. We presented a first principle model, which includes a numerical exact solution of the time-dependent Schrödinger equation [1]. All nuclear rotational and vibrational states and the coupling between them are included. The simulation aims to describe the full physical process that initiates at a finite temperature. Therefore, the initial conditions of the system were set to be thermal and to include different rovibrational states. The simulation outcomes are analogous to experimental observables, such as the momentum angular distribution of the photo-fragments.

The random phase thermal wavefunction (RPTW) method is used to overcome the challenge of the large Hilbert space. It replaces the density operator calculations by a finite sample of random phase thermal wavefunctions. We developed methods to calculate the full asymptotic photo-fragment distribution, and studied the convergence of the calculation with respect to the number of RPTW employed. Typically, in the RPTW theory the convergence of the observables scale with the number of realizations, K, and the Hilbert size, $N_s$, as $\sim \frac{1}{\sqrt{K}} \cdot \frac{1}{\sqrt{N_s}}$ [2]. We want to investigate the prefactor of this scaling, or particularly know what the number K of RPW that is required to converge a specific observable to experimental accuracy [3]. We used the freedom of setting the model to explore fundamental processes and simplify the full complexity into a two-electronic-state system. The simplified model enables clear and informative benchmarking before going down the rabbit hole of the complete and detailed simulations of the photo-dissociation process. The model complexity will be increased by steps. The modular construction will allow to sort out the different contributions to the process and allow direct analysis of experiments.

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# Investigating the Interstellar Chemical Complexity through Discharge Experiments and Rotational Spectroscopy

Amanda L. Steber[1], Cristóbal Pérez[1], Wenqin Li[1], Alberto Lesarri[1]

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The characterization of the molecular inventory in interstellar and circumstellar environments is a pressing problem in Astrochemistry. The identification of the molecular species present in these astronomical environments informs us about the chemistry that is occurring, and by proxy the chemistry that could lead to the formation of biologically relevant molecules. The current inventory of molecules in space contains over 260 species, mostly characterized through rotational spectroscopy, and it is predominantly comprised of small (typically <10 atoms) compounds containing C, H, O, and N atoms. Many of these molecules are terrestrially unstable species, including ions and radicals. However, despite the fact that larger species, such as fullerenes and polycyclic aromatic hydrocarbons (PAHs), have been recently detected, the catalogue of molecular species is far from complete, especially considering the enhanced sensitivity of modern radio telescopes.

To contribute to our understanding of astrochemical, an electrical DC-discharge nozzle has been used to generate terrestrially unstable species, that are later stabilized in a cooled supersonic expansion. While the conditions within the discharge are very different from those in interstellar environments, discharge experiments produce short-life molecules that can be detected in the low-density astronomical environments. These new species may be key intermediate species in chemical processes leading to the formation of biologically relevant compounds, which in turn might have been present in the formation of planetary systems. In our experiment we have paired an electrical discharge nozzle with a broadband microwave spectrometer to measure the resulting products of the discharge of PAHs and/or small organic compounds previously identified in the molecular inventory. The rotational spectra from new species are then used for astronomical searches with radio telescopes. Furthermore, we investigate probable reaction pathways that these species could participate in through quantum chemical calculations and astrochemical models, providing a global view of the matter cycle in the interstellar medium.

# Non-trivial fragmentation on photoionized Diketopiperazines: new insights on prebiotic chemistry

Darío Barreiro-Lage[1], Paola Bolognesi[2], Jacopo Chiarinelli[2], Robert Richter[3], Henning Zettergren[4], Mark H. Stockett[4], Lorenzo Avaldi[2] and Sergio Díaz-Tendero[1,5,6]

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Several scientific theories have been proposed for the conundrum of the origins of life on Earth: the panspermia theory, the iron-sulphur world, the RNA world, the ‘proteins first’ theory, etc. But, at the end, these theories still do not explain the formation of complex biological systems, as they just rely on arbitrary or random processes leading to bigger proteins or nucleic chains from inner or outer space. Considering the emergence of life as a process of evolution in a dynamic chemical network[1], alpha-amino acids and random oligopeptides shall have played an important role from the very beginning, acting as prebiotic ‘seeds’ that could lead to the formation of more complex systems. Thus, shedding light on the mechanisms of production of prebiotic building blocks is of paramount importance to understand the abiotic synthesis of relevant biologically active compounds. In this work it will be shown that for a possible elongation of the peptide chain, two main agents must be present: a 'seed' and a reactive moiety.

A combined experimental and theoretical study of the interaction of VUV radiation with three different 5-diketopiperazines (DKPs): cycle-alanine-alanine[2,3], cycle-alanine-glycine and cycle-glycine-glycine have shown that, after ionization, these molecules present very interesting fragmentation paths and, contrary to what might be expected, notably different from each other. Photoelectron spectrum and photoelectron–photoion coincidence (PEPICO) measurements combined with theoretical simulations have revealed that, after molecular decomposition, these 2,5 diketopiperazines can produce small aziridin intermediates that could act as prebiotic ‘seeds’, as well as reactive oxazolidinone intermediates.

Furthermore, theoretical simulations reveal that the interaction of these intermediates, can lead to the elongation of the peptide chain. These results may explain how DKPs could have, on one hand, survived hostile chemical environments and, on the other, provided the seed for amino acid polymerization.

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# A theoretical journey from DNA building blocks to bioreceptors

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In this perspective talk, I will focus on how theoretical and computational chemistry can obtain spectroscopic and dynamical information from biomolecules under light irradiation. In contrast to gas phase experiments, biomolecules are in solution, which poses a grand challenge for theoretical chemistry. By the hand of few examples from DNA building blocks to bioreceptors, I will illustrate how in one can predict how solution changes absorption, emission, relaxation mechanisms and charge transfer properties. The methods of choice are multiscale quantum mechanics/molecular mechanics (QM/MM), molecular dynamics and excited state nonadiabatic dynamics.

# Nanofabrication with layers of mass-selected ions

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Advances in the design of micro- and nanoscale material on surfaces have revolutionized modern technology. However, interdisciplinary research combining chemistry, physics and engineering continues to face the challenges of (i) tuning the precise elemental/molecular composition of a material required for a targeted property and (ii) assembly of such defined material with control over shape and structure on a surface suitable for applications. While convincing approaches like Molecular Beam Epitaxy (MBE) or Atomic Layer Deposition (ALD) have been established and extensively studied for volatile deposition precursors, the class of complex molecular ions remained widely untouched so far with respect to nanofabrication. Such ions provide a variety of technologically relevant properties (e.g., they can act as photosensitizers [1] or catalysts [2]) but found little attention for thin layer preparation due to the typically low volatility of ionic compounds.

In this contribution, the method of ion soft-landing will be introduced as a tool for preparation of thin layers of organometallic ions that can act as suitable substrates for subsequent particle-induced nanostructuring. A set of first experiments will be presented showcasing the capabilities of modern ion soft-landing for generation of relevant quantities of mass-selected material within highly affordable timeframes. This is enabled by bright Electrospray Ionization (ESI) sources and ingenious ion transfer optics [3]. The obtained layers of organometallic ions were then subjected to electron beam processing in order to fabricate micro- to nanostructures out of the deposited material (see Fig. 1).

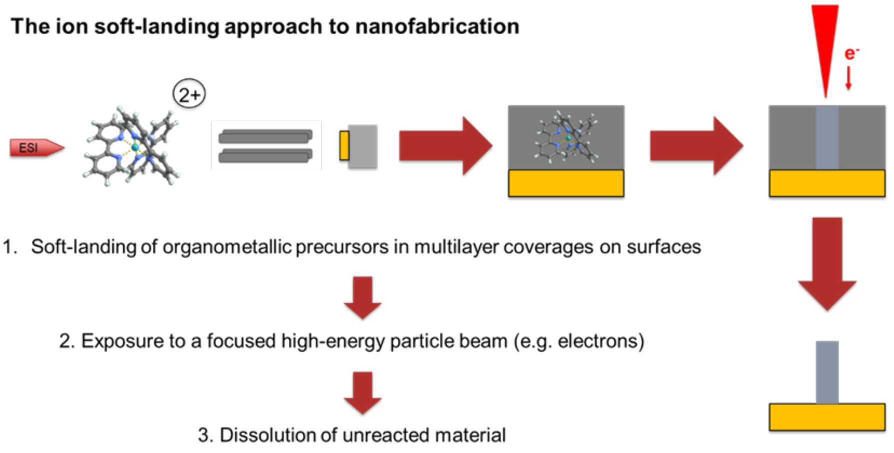

*Figure 1. Ion soft-landing approach to nanofabrication on the example of mass-selected $(EtCp)_2Ru$ ions.*

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# Using theory to pull back the curtain on experiment

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The study of chemistry is underpinned by the desire to understand reactivity. In nature, reactivity is ubiquitous with light and/or electron driven processes. Historically, both experimental and theorical studies of reaction dynamics have been limited by a size/accuracy compromise. This has restricted high accuracy studies to isolated reactive moieties in the gas phase, where intrinsic dynamics can be explored and understood in detail. To build fundamental understanding of the 'how and why' of chemistry it is necessary to use this bottom-up approach before moving to include the native reactive environment. Experiment can be used to observe the chemistry of systems, while theory can interpret these observables.

Anions require particularly careful handling computationally, requiring the use of non-conventional electronic structure methods to model their assortment of exotic states. Through building a computational toolkit I have been able to use novel applications of computational chemistry to gain new insight into the observables of anions in the gas phase, alongside anion photoelectron spectroscopy experiments.

In this talk I will showcase the need for this computational toolkit, showing how it can aid confident interpretation and assignment of experimental signatures that would otherwise have been too ambiguous to understand.

**Relevant publications**

1. C. S. Anstöter* and J. R. R. Verlet, Gas-phase Synthesis and Characterisation of the Methyl-2,2-dicyanoacetate Anion Using Photoelectron Imaging and Dipole-bound State Autodetachment, *J. Phys. Chem. Lett.*, 2020, **11**, 6456–6462.
2. C. S. Anstöter* and J. R. R. Verlet, Modeling the Photoelectron Angular Distributions of Molecular Anions: Roles of the Basis Set, Orbital Choice, and Geometry, *J. Phys. Chem. A*, 2021, **125**, 4888–4895.
3. C. S. Anstöter, C. R. Dean and J. R. R. Verlet, Sensitivity of Photoelectron Angular Distributions to Molecular Conformations of Anions, *The Journal of Physical Chemistry Letters*, 2017, **8**, 2268–2273.

# Diamond(doid)s are a physicist's best friend

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Diamondoids are a class of carbon nanomaterials based on carbon cages with well-defined structures formed by C(sp3)-C(sp3)-hybridised bonds and fully terminated by hydrogen atoms. All diamondoids are variants of the adamantane molecule, the most stable among all the isomers with formula $C_{10}H_{16}$. A recent series of photoionisation experiments have been performed in various large-scale facilities to reveal the fragmentation dynamics of adamantane cations.

The initial experiment was done at Lund University using femtosecond XUV pulses produced via high-order harmonic generation and ion/electron spectroscopy [1]. As a main result, we were able to show that the doubly charged adamantane molecule is metastable and will spontaneously dissociate. However, preceding dissociation, the cage structure will open and hydrogen migration(s) will occur (see Fig. 1). In addition, we were able to assess the energetic picture of the dication processes thanks to the measured ion and electron kinematics combined with theoretical calculations, allowing us to discuss the internal energy distribution of the system.

To delve deeper into adamantane's properties we recently performed a set of complementary studies such as time-resolved photoionisation experiments using pump-probe techniques (XUV-IR at the Lund Attosecond Science Center and XUV-XUV at the Free-electron laser FLASH2), core-ionisation measurements at the synchrotron SOLEIL (FR) and time-dependent photoabsorption spectroscopy at the cryogenic ring DESIREE (SE) from which preliminary results will be presented.

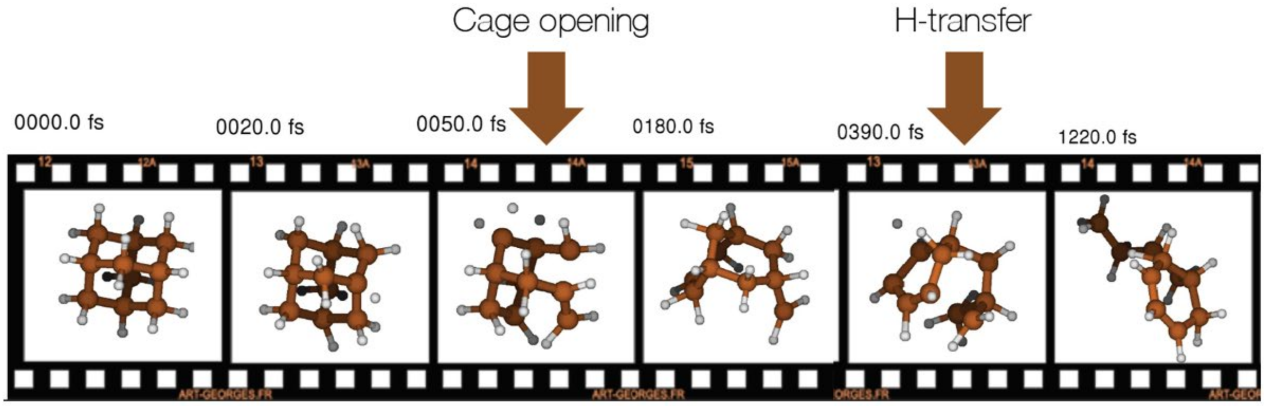

Figure 1: Molecular dynamics simulations showing the opening of the carbon cage.

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# Histidine tautomerism modulated misfolding mechanism of prion protein: new insights from replica exchange molecular dynamics

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The accumulation and conformational transition of normal prion protein (PrP$^{C}$) into the pathogenic scrapie form (PrP$^{Sc}$), which can act as a seed to induce prion amyloid fibril formation, is believed to be a central event in prion diseases. No effective treatment has been identified for prionopathies. Earlier study highlights that the monomeric prion may play a key role in oligomer formation during disease development. Herein, for the first time we explored the structural properties of the huPrP (125−160) monomer with different histidine states (δ; N$^{\delta 1}$-H, and ε; N$^{\varepsilon 2}$-H) using extensive replica-exchange molecular dynamics (REMD) simulation. Interpreting the organizational properties and misfolding procedure is a challenging task because two tautomeric forms can occur in the free neutral condition. Atomistic simulation results have shown that the toxic εδ (carrying one ε and one δ histidine) and δδ tautomeric isomer (involving several and broader local minima) had the highest α-helical formations, with values of 21.11% and 21.01%, respectively, and may have a strong impact on the structural behavior of a prion monomer. The residues aspartate 20 (D20)−asparagine 29 (N29) and isoleucine 15 (I15)−histidine 16 (H16), D20−arginine 27 (R27) as well as N29 produced α-helix with the highest probabilities in the δδ and εδ tautomer, respectively. The helices appeared as thick bands along the main diagonal in the tautomers' contour maps. Furthermore, the fluctuation and hydrogen bond analysis results established that the histidine tautomeric states influence intratautomer residual flexibility and connections, which can affect the PrP$^{C}$−PrP$^{Sc}$ configurational transformation. Altogether, we proposed histidine tautomerization hypothesis that constitutes an excellent prospect for inducing understanding of molecular pathogenesis of prionopathies and may assist in the design of a good therapeutic agents.

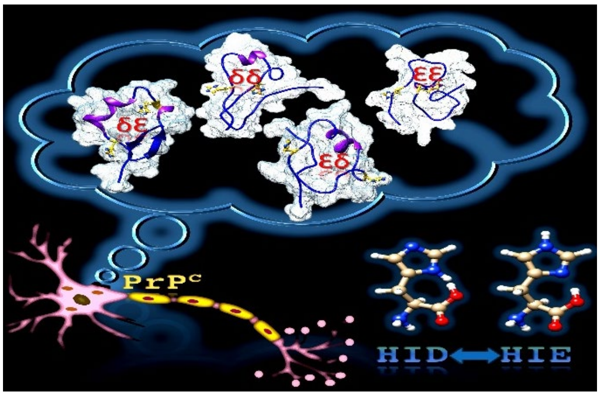

***Figure. The Contribution of the Novel Histidine Tautomerism Hypothesis to the Understanding of Neuro Diseases***

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# Ion dynamics in laser-irradiated helium gas around a nanoparticle

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Atomic clusters and substrate-free nanoparticles provide an attractive target for investigation and control of many-body dynamics on ultrafast time scales. Among the appealing phenomena reported in NIR-laser-irradiated clusters are resonant absorption or ion and electron acceleration to surprisingly high energies [1]. In the XUV domain, formation and dynamics of nanoplasmas [2] or correlated electronic decay [3] are of high interest.

To interpret the experimental results, an isolated nanoparticle in vacuum is generally used as a model target. However, in many experiments, the nanoparticles are surrounded by a gaseous atmosphere, which can considerably affect the overall dynamics of the laser-irradiated sample.

We investigate the interaction of CsCl nanoparticles (diameters of few 100 nm) in a helium atmosphere with intense lasers (either NIR laser with a peak intensity of $2\times10^{15}$ Wcm$^{-2}$, or an XUV beam). By detecting and analyzing ions and electrons produced in the laser-nanoparticle interaction, we unravel the ion acceleration mechanisms both with and without the nanoparticle.

Already without the nanoparticle, helium ions are accelerated to energies of around 100 eV [4]. When the nanoparticle is injected into the focal volume, helium ions can gain energies of up to 1 keV. The energy of helium ions exceeds energies of nanoparticle ions, which originate in a much higher density plasma [5]. We explain the ion acceleration processes by electrostatic models. Without the nanoparticle, a charge separation drives the ion explosion, while with a nanoparticle, an electric field around the ionized nanoparticle provides additional ion acceleration.

The mechanisms presented here should be universal to many types of targets, eg. clusters, helium nanodroplets, biomolecules or targets produced by laser ablation irradiated by photon energies ranging from NIR to XUV.

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# *Ab initio* characterization of noble gas containing molecules with astrochemical interest: data-driven intermolecular potential and spectroscopic data

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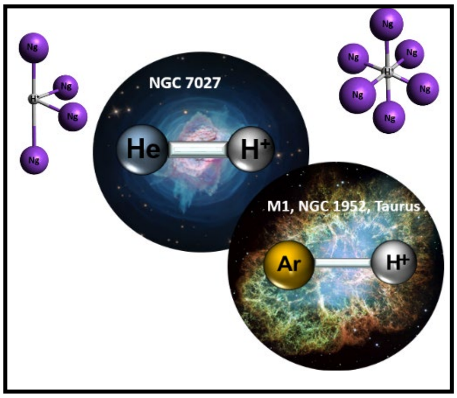

**Figure 1.** *Visual description of HeH$^+$ and ArH$^+$ discoveries [1,2] , as well as higher-order noble gas containing molecules.*

For a long time, the interstellar medium (ISM) has been considerate inhospitable environment to chemical compounds due to the extreme conditions that characterized it and, only a few molecules could be form. However, this point of view has changed dramatically in the last decades and more than 240 compounds have been observed in the space. Several of the molecules formed are "unconventional" and quantum chemistry is an exceptional tool to explore and understand their properties especially in those cases in which experimental is short-coming. Moreover, the growth of accurate modern quantum chemical approaches, as well as integration of new technologies in data science have the potential to improve the decision making in astrochemistry/physics projects. The purpose of this work is to explore trends and models for data science research, in order to propose action protocols for carrying out computational quantum chemistry investigations providing astro-chemically relevant data for identifying new noble gas containing molecules potentially detectable in the ISM. More concretely, the most fascinating discoveries in the recent years in the field were the recorded presence of ArH$^+$ and HeH$^+$ [1] in the ISM (see Fig.1). Therefore, our research is focused on the computational characterization of such Ng$_n$H$^+$ species, starting from high-level electronic structure calculations [2], combining with RHKS approach for a global representation of the underlying potential interactions in order to understand the chemical bonding and electron sharing of the simplest noble gases hydride cations cluster [Ng$_2$H]$^+$, and further to provide spectroscopic data through quantum chemical tools [3,4] (see Fig.2). Such accurate predictions on energetics and spectroscopic properties could facilitate the astrochemical detection of such noble gas compounds in some ISM regions. In the same way, the comparison with the previously reported values indicates that the present data could serve as a benchmark for future on higher-order cationic [Ng$_n$H]$^+$of astrophysical interest.

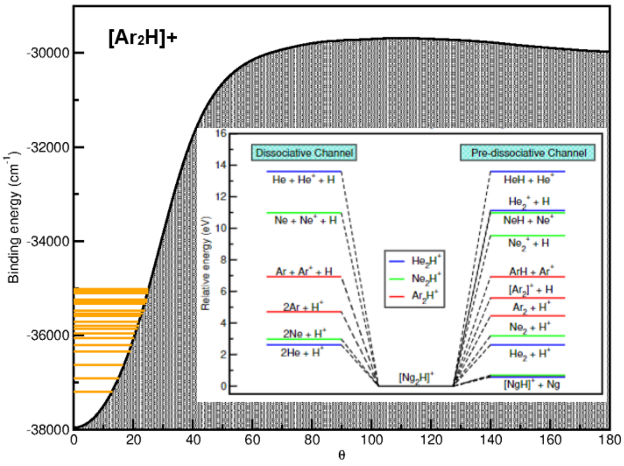

**Figure 2.** *Minimum potential energy path together with bound vibrational levels, as well as energies of dissociative and predissociative channels of Ar$_2$H$^+$ using the CCSD(T)/CBS [56] RKHS PES.*

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# Investigating the electrolyte-to-metal transition in liquid alkali-metal ammonia solutions

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Liquid ammonia shows many characteristics similar to water, namely its ability to establish a hydrogen bond network, to dissolve salts in order to form an electrolyte solution or to be the solvent for redox processes such as the Birch reduction. Unlike water, which reacts very vigorously upon contact with alkali metal, liquid ammonia stabilizes the dissolved alkali cations and the excess electrons for extended periods of time. This offers the possibility to study the energetics and reactivity of 'naked' electrons in solution. One classic phenomenon is the electrolyte-to-metal transition: at low alkali metal concentrations a dark blue solution containing solvated electrons forms. Upon increase of alkali metal concentration its colour changes into bronze-golden undergoing a phase-transition into a liquid metal solution which is accompanied by an increase of the electric conductivity by orders of magnitude. Recently, electronic structure changes happening during the phase-transition have been measured for the first time. Those will be discussed as well as analogies to the transition of semi-conductor becoming metals upon doping with impurity atoms as observed in solid-state physics.

# Hydrated Metal Ions: Nanolaboratories for modelling of elementary (photo)chemical processes

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Hydrated metal ions in the gas phase, $M^+(H_2O)_n$, $n \approx 1$–100, might be used to elucidate various elementary processes with an unprecedented level of detail. For example, we might follow cluster isomerization, reactions with other molecules, the shift of the excitation energy or photochemical decomposition channels along step-by-step hydration. At the same time, these systems are well defined and small enough to be treated by quantum chemical methods. Comparing reactivity and photochemical properties of different metal ions with various hydration degrees, we might obtain insight into trends within the periodic table of elements.

Here, I will focus on our recent work on several hydrated metal ions including $Mg^+$, $V^+$ and $Al^+$. The systems were prepared experimentally within Fourier Transform Ion Cyclotron Resonance (FT-ICR) mass spectrometry, their (photo)chemical properties were probed through irradiation with IR and UV lasers. To understand the experimental results, we used both ground state and excited state quantum chemical approaches on different levels of sophistication.

I will show that photochemistry of the investigated hydrated metal ions differs considerably from their ground state chemistry, with a wide variety of photochemical phenomena including internal conversion, intersystem crossing, photoisomerisation and photodissociation. In particular, the photochemistry of the vanadium cation with about 200 electronic states within 3 eV from the ground state energy will be discussed as a challenge for photodynamics. I will also focus on symmetry breaking as a useful tool to understand main features of hydrated metal ions photochemistry.

# Quantum degenerate gas of polar molecules

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A degenerate Fermi gas of polar molecules [1] sets the stage to explore novel molecular dynamics. A precisely controlled electric field is applied to tune the elastic dipolar interaction by orders of magnitude while suppressing reactive losses. Efficient dipolar evaporation leads to the onset of quantum degeneracy in two-dimensional optical traps [2]. The electric field tuning of the rotational energy also produces sharp collision resonances, giving rise to three orders-of-magnitude modulation of the chemical reaction rate [3].

The precise control of electric field has also allowed us to prepare and address isolated, individual two-dimensional layers of molecules with arbitrary choices of rotational state. We study exchanges of rotational angular momenta between molecules of neighboring layers through long-range dipolar interactions, demonstrating quantum-state engineered stereo chemical reaction [4]. Meanwhile, these interacting molecules in 2D are used to realize a tunable spin Hamiltonian for quantum magnetism.

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# Towards collisional cooling of polyatomic molecules

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The last decades have been the time of intensive development of chemistry and physics of ultracold matter, both in terms of theoretical description and experimental methods [1]. Currently, finding effective methods of cooling polyatomic molecules has become a significant challenge. Gaseous formaldehyde ($H_2CO$) has recently been optoelectrically cooled to submillikelvin temperatures [2]. The next step of lowering temperature may be achieved by immersion of polyatomic molecule in an ultracold atomic bath (sympathetic cooling). Here, we theoretically investigate intermolecular interactions and chemical reactions in ultracold mixtures of formaldehyde in a ground electronic state with alkali-metal (Li, Na, K, Rb, Cs) and alkaline-earth-metal (Be, Mg, Ca, Sr, Ba) atoms in ground and first excited electronic state. We applied highly correlated *ab initio* electronic structure techniques to compute potential energy surfaces (PES) for selected geometries of the system [3]. The two-dimensional surfaces for $Rb+H_2CO$ are expanded into the Legendre polynomial basis and can be employed in further scattering calculations. Scalar relativistic effects for heavy metal atoms are included via small-core pseudopotentials [4]. We calculated long-range van der Waals induction and dispersion coefficients within the perturbation theory. We analyzed possible channels for reactive collisions based on the energetics of stationary points of reactants and transition states. The following research project is a first step toward effective modelling of sympathetic cooling and ultracold controlled chemistry for neutral polyatomic molecules with ultracold atoms.

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# Trapped chiral molecular ions for probing weak force parity violation

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The symmetry between left- and right-handed chiral molecules is predicted to be broken by the weak interaction. Some theories suggest that this small energy difference has seeded the homo-chirality observed in nature, though such predictions are controversial. We are building a new experiment aimed at observing weak force parity violation (PV) for the first-time molecules. We will use the charged version of chiral molecules which can be easily trapped providing long interrogation times. We will present our plans to extract the PV signature through Ramsey spectroscopy on a mixed racemic ensemble of the trapped molecular ions.

# Chemistry and physics in multiply charged helium nanodroplets

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Clusters and nanoparticles have size-dependent physical and chemical properties, which are also very different from the properties of corresponding bulk materials. In past decades, these unique cluster properties have attracted a lot of attention in a range of fields from basic science to applied chemistry. However, as E.C. Tyo and S. Vajda have pointed out in their famous review article: "*The limiting factor in all cluster studies is creating a sufficiently high concentration of the desired species and separating them from the overall distribution formed during cluster generation.*"[1]

In the present study, we demonstrate the possibility of forming singly charged clusters via the pickup of various dopants into multiply charged superfluid helium nano-droplets with cluster size distributions that are much narrower compared to conventional gas-phase methods.[2] We have achieved size distributions narrower than Poisson, for example, for gold and silver clusters. Moreover, we are able to tune, which cluster size is the most abundant. To understand which physical parameters are responsible for such narrow cluster size distributions, we have made simulations, which nicely fit the experimental data. This knowledge will help in future experiments to produce any desired cluster size with the highest efficiency.

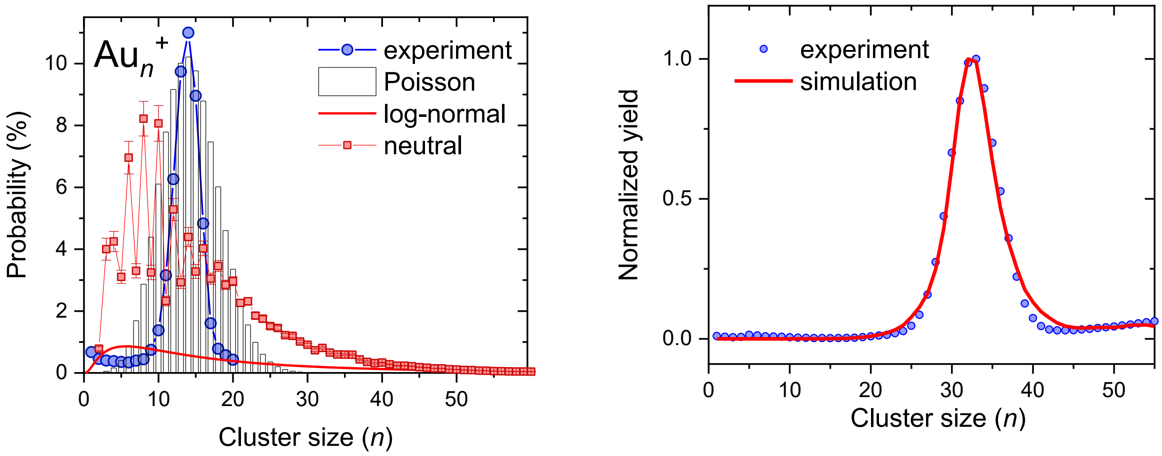

**Figure:** *Left:* The size distribution of gold cluster ions obtained upon pickup into charged (blue circles) and neutral (red squares) He nanodroplets. The bar graphs and red trace represent corresponding Poisson and lognormal distributions. *Right:* The blue circles represent the size distribution of gold cluster ions and the red line is the result of a simulation.

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# Quantitative study of enantiomer-specific state transfer

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The non-superimposable mirror images (enantiomers) of a chiral molecule can have vastly different chemical properties while having mostly identical physical properties. This makes enantiomer-specific control of a chiral molecule in the gas phase inherently difficult. Recently, the enantiomer-specific state transfer (ESST) method was developed using tailored microwave fields [1]. This method allows to populate or depopulate a rotational state of a chosen enantiomer, providing a way of quantum-controlled chiral separation. Previously, the transfer efficiency of ESST was limited by thermal population [1,2] and by spatial degeneracy [3] of the involved energy levels. To address these prior limitations, we developed a new experimental scheme which increases the state-specific enantiomer-enrichment by more than an order of magnitude compared to previous studies [4]. Notably, our scheme enables a quantitative comparison between experiment and theory for the first time. In our study with the molecule 1-indanol, we choose the simplest possible ESST triangle which includes the absolute ground state level, $|J_{K_aK_c}\rangle=|0_{00}\rangle$. Details of the experimental scheme as well as results will be discussed in the presentation.

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# Recent results on the ion molecule reactive scattering

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We study kinematically complete ion-molecule reaction dynamics using a crossed-beam setup with velocity map imaging (VMI) [1]. By studying the differential cross-sections of the ionic reaction products, obtained from the VMI data, we gain insight into the microscopic details of the low energy ion-molecule collision mechanisms [2-4]. Here we will report on two recent results regarding ion-molecule reactive scattering. Firstly, we have investigated the $F^- + CD_3I$ reaction in the relative collision energy range from 0.7 to 2.3 eV. Further, the results are compared with the hydrogenated counterpart $F^- + CH_3I$ reaction [5] as well as quasi-classical trajectory (QCT) simulations from the Czakó group [6]. The $F^- + CH_3I$ reaction shows a significant large-impact parameter contribution in the $S_N2$ channel, which is absent for its deuterated counterpart, manifests itself as an enhancement of forward-scattered events in the product angular distribution. The simulations can fully capture the $S_N2$ dynamics in the reaction with $CD_3I$, while large-impact parameter events from $F^- + CH_3I$ cannot be reproduced. Such a discrepancy between experimental and theoretical work might hint toward a quantum effect that cannot be captured by QCT simulations. Secondly, we also report on very recent results on the reactive scattering of $CH_3I$ with $O^-$ radical anions.

Presently we are in the process of making a new, improved version of the present experimental setup in terms of higher resolution and repetition rate. We will present the design concepts and simulations for the experimental setup that uses coincidence detection of both the ionic and neutral products after the reaction, utilizing a laser ionization scheme.

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# The Changes in Electronic Structure of PAH Cations Induced by Hydrogenation

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Polycyclic aromatic hydrocarbons (PAHs) are widely distributed in interstellar medium (ISM) [1] and contribute to molecular hydrogen formation [2]. Thermal atomic hydrogen beam attaches to gas phase PAHs with magic number [3] and a identified sequence [4]. In order to understand deeply changes of electronic structure caused by hydrogenation and photo-stability of PAH, soft X-ray absorption spectra in PAH cations (including anthracene, pyrene, hexahydropyrene, triphenylene, and coronene) and their hydrogenated counterparts were studied in combination of experiments and theoretical calculations. The PAH cations and hydrogenated PAH cations were trapped in a cryogenic linear radiofrequency (RF) ion trap and interact with monochromatic X-rays around the carbon K-edge. Photo-products were collected and recorded by a time-of-flight (TOF) mass spectroscopy as a function of photon energy. To explain and interpret experimental data, a state-of-the-art time dependent density functional theory (TDDFT) calculation was performed based on short-range corrected (SRC) functional.

The reduction of gap between HOMO-LUMO is revealed by a red shift of transition from 1s to $\pi^*$ resonance in spectra. Non-dissociative ionization, $H/H_2$ loss and fragmentation of carbon backbone compete to each other as major relaxation channels. The carbon backbone is protected by H loss and non-dissociative ionization. The photo-products induced by X-rays depend on the size and geometry of PAH. For larger and more symmetrical PAHs, for instance coronene, additional hydrogen decreases the fragmentation cross section of carbon backbone. However, non-dissociative ionization is suppressed via hydrogenation for pyrene. As a result, the PAHs with big size incline to survive and facilitate $H_2$ formation exposed to radiation fields in ISM.

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# Quantum control of ultracold ion-atom collisions

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Hybrid systems of laser-cooled trapped ions and ultracold atoms combined in a single experimental setup have recently emerged as a new platform for fundamental research in quantum physics and chemistry [1]. Reaching the ultracold s-wave quantum regime has been one of the most critical challenges in this field for a long time. Unfortunately, the lowest attainable temperatures in experiments using the Paul ion trap are limited by the possible rf-field-induced heating related to the micromotion. In my talk, I will present how, in collaboration with experimental groups of Rene Gerristma in Amsterdam and Tobias Schaetz in Freiburg, we have overcome the micromotion limitation, reached the quantum regime, and demonstrated the quantum control of ultracold ion-atom collisions, all for the first time. In Amsterdam, buffer gas cooling of a single 171Yb+ ion in a Paul trap with ultracold 6Li atoms to the quantum regime of ion-atom collisions was realized, and a deviation from classical Langevin theory was observed by studying the energy dependence of the spin-exchange dynamics, being the first observation of shape resonances in ion-atom collisions [2]. In Freiburg, magnetically tunable Feshbach resonances between a single 138Ba+ ion and 6Li atoms were demonstrated by measuring enhancement of three-body recombination losses and sympathetic cooling rates [3]. The experimental efforts were guided and confirmed by our electronic structure and multichannel quantum scattering calculations, including the first determination of ion-atom scattering lengths. The achieved quantum control of ion-atom collisions opens the way for a plethora of applications in studying the few-body and many-body problems of a single ionic impurity in ultracold atomic or molecular gases.

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# Towards controlled reactive collisions

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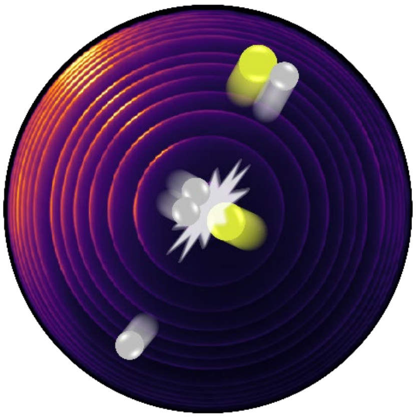
One of the important goals in physical chemistry is to get a complete understanding of fundamental molecular processes that underlie chemistry. Our aim is to investigate and control molecular scattering processes in extremely high detail and in unexplored energy regimes.

The combination of Zeeman deceleration and Velocity Map Imaging in a crossed molecular beam setup is a powerful tool to study molecular collisions. The decelerator allows for precise control over an atomic or molecular beam, while Velocity Map Imaging in combination with near-threshold ionization enables us to accurately probe the velocity vectors of the scattered products. This combination of techniques therefore enables scattering experiments with extraordinary resolution, revealing intimate details of molecular collisions that are washed out otherwise.

Up to now, we used this experimental approach to investigate *inelastic* collisions, for instance between carbon and helium atoms [1], or carbon atoms and hydrogen molecules. Our high-resolution experiments allowed for a detailed investigation of scattering resonances and their effect on the angular distributions of the scattered C-atoms for both systems.

Recently, we started using our approach for investigating *reactive* collisions. We aim to measure the energy dependence of state-to-state differential cross sections in order to provide an extremely sensitive test for potential energy surfaces and scattering calculations used to describe the reaction dynamics.



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# Bound electron enhanced radiosensitisation of nimorazole upon charge transfer

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Nimorazole (NIMO ≡ $C_9H_{14}N_4O_3$), is a chemical compound that has been widely used as an efficient hypoxic cell radiosensitizer in head and neck squamous carcinoma due to its low toxicity [1]. Its ability to scavenge low-energy electrons (LEEs) has been recently shown to be very efficient in producing a non-dissociate parent anion with a considerable large cross-section of $\sim 3\times10^{-18}$ m$^2$ [2,3], while dissociative electron attachment has been shown to be a minor reaction channel which is suppressed upon hydration [1]. While associative electron attachment may contribute to NIMO's radiosensitising effect, within the biological environment, electron transfer processes (redox reactions) may prevail and so these may seem more appropriate to describe the underlying molecular mechanisms of such chemical compounds and their role as radiosensitizers. Thus, we have initiated more than a decade ago an investigation methodology to explore key selected radiosensitizers by charge transfer in atom-molecule collision experiments, e.g. halouracils [4].

The crossed molecular beam setup used to investigate collisions of neutral potassium (K) atoms with neutral nimorazole (NIMO) molecules, has been described in detail elsewhere [5]. Briefly, an effusive target molecular beam crosses a primary beam of fast neutral K atoms and the product anions are analysed using a reflectron (KORE R-500-6) time-of-flight (r-TOF) mass spectrometer. The K beam is produced in a resonant charge exchange chamber from the interaction of $K^+$ ions from a commercial potassium ion source (HeatWave, USA), in the range of 20 to 1000 eV in the lab frame, with gas-phase neutral potassium atoms from an oven source. The TOF negative ions spectra shows a rich fragmentation pattern, yet the most intense are assigned to the nitrogen oxide ($NO_2^-$) and a non-dissociate parent ($NIMO^{\bullet-}$) anions. Moreover, $K^+$ energy loss spectrum revealed for the first-time important information on the vertical electron affinity of the most accessed negative ion states in such collisions [7]. Given that nitroaromatic chemical compounds bind selectively to hypoxic cells, reduction of the $-NO_2$ group to the $-NH_2$ group occurs through a series of reactive intermediates, by sequential addition of an electron and protonation [6]. These electron transfer results show that such $NO_2$ reduction is an efficient process to the bare molecule in the gas-phase [7]. Further details supported by state-of-the-art quantum chemical calculations of the molecular orbitals will be given at the meeting.

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# MS SPIDOC: mass spectrometry meets single particle imaging

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Native mass spectrometry (MS) enables the ionization and transfer of structurally intact non-covalent protein complexes into the gas-phase. As such, it is a perfect tool to study proteins and their assembly intermediates in a mass and conformation specific manner. However, structure follows function, and the structural information that can be gained with techniques like top-down MS or ion mobility is limited. Accordingly, other experimental approaches such as X-ray diffractive imaging are necessary to get a full understanding of the proteins and their assemblies.

MS SPIDOC (Mass Spectrometry for Single-Particle Imaging of Dipole Oriented Protein Complexes) is a Horizon 2020 funded research and innovation program [1] aiming at the combination of both experimental techniques. In particular, well-established methods from MS like *m/z* selection, ion trapping or ion mobility are adapted as part of the sample delivery system for X-ray diffraction. In contrast to conventional diffractive imaging of crystallized proteins, the proteins here are delivered as single particle without the need for crystallization. This increases naturally the requirement to the X-ray source. Thus, single-particle X-ray diffractive imaging (SPI) is only conducted at X-ray free electron lasers [2], the worlds brightest X-ray sources in the world.

This contribution will highlight the ongoing efforts of the MS SPIDOC consortium to develop this sample delivery system for the use at beamlines of the European XFEL [3]. The current state of the designing and manufacturing of the instrument prototype will be presented as well as the results of the first testing of individual component modules. Furthermore, theoretical simulations as well as experimental device design for particle dipole orientation in strong electric fields will be previewed.

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# Size effects of tantalum cluster cations on simultaneous activation of methane and carbon dioxide

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Global warming is likely to represent the greatest challenge faced by our generation. Therefore reducing greenhouse gas emissions, notably methane and $CO_2$, is essential for achieving set climate goals. Capturing these molecules from certain emitters and converting them into valuable chemicals are the most promising ways to prevent their release into the atmosphere from processes, in which their formation cannot be avoided (e.g., in cement or steel production or agriculture).

Modern approaches do consider novel thermal processes as catalysis with atomic precision by applying single atom and size selected particles but also photocatalytic reactions, with the latter enabling to overcome thermodynamic limitations and conduct the reactions at room temperature. In addition to these studies, the work on the $Ta^+$-mediated single-atom catalysis of $CO_2/CH_4$ coupling by group of H. Schwarz [1], and our recent publications of the separate activation of both molecules on atomically precise $Ta^+$-clusters [2-4], have motivated us to perform the research on conversions of $CO_2$ and $CH_4$ on two different tantalum cations, namely $Ta^+$ and $Ta_4^+$. While both compounds indeed enable the coupling of these molecules, they also reveal stark differences in product formation. Product analysis and reaction kinetics indicate a predisposition of the tetramers for C–O coupling, whereas atomic cations enable C–C coupling. Aided by DFT-calculations of the reaction thermochemistry and our previous structural analysis of the intermediates [5], we identify peculiar differences, which are assigned to being responsible for the change in the course of the coupling reaction.

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# DNA nanotechnology: from coarse-grained modeling to experimental realization

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DNA nanotechnology uses designed DNA strands to assemble nanoscale structure and devices. These structures can contain up to tens of thousands of nucleotides, posing a major challenge to computational modeling of such systems due to their size as well as rare events (creation or breaking of base pairs) during their assembly. Here, we present multiscale coarse-grained models and design tools that have been specifically developed for simulations of DNA and RNA nanostructures. One of the main challenges for design of self-assembling structures is to maximize the yield of the desired target structure and avoid undesired alternative structures that the system might also assemble into. We will present our new design pipeline for assembly of multicomponent DNA nanostructures and show its application to design of 3D metamaterial lattices geometries.

# Accurate global $^3A''$ potential energy surface for the O+C$_2$($^1\Sigma_g^+$,$^1\Pi_u$) reaction

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The reaction between O($^3$P) and C$_2$ reaction plays an important role in combustion processes, soot formation, and is relevant to describe the chemistry of molecular clouds and dying carbon stars.*[1][2]* It is also important in the formation of polycyclic aromatic hydrocarbons (PAH) and carbon nanostructures.*[3]* In spite of this, its dynamics has been barely studied.

From a computational point of view, the study of the O($^3$P) + C$_2$ reaction is particularly cumbersome. On the one hand, in the reactants asymptote we deal with two open-shell fragments. On the other hand, the energy difference between the ground and the first excited state of C$_2$ ($^1\Sigma_g^+$ and $^3\Pi_u$) is less than 0.09 eV, so both are populated at thermal energies. Accordingly, many configurations and electronic states have to be considered. Here, we present the first $^3A''$ potential energy surfaces (PES) of the O($^3$P) + C$_2$($^1\Sigma_g^+$,$^3\Pi_u$) reaction. The ab-initio energies have been calculated at the MRCI(+Q)/aVTZ level, and the PES are fitted using the many-body expansion procedure. *[4]*

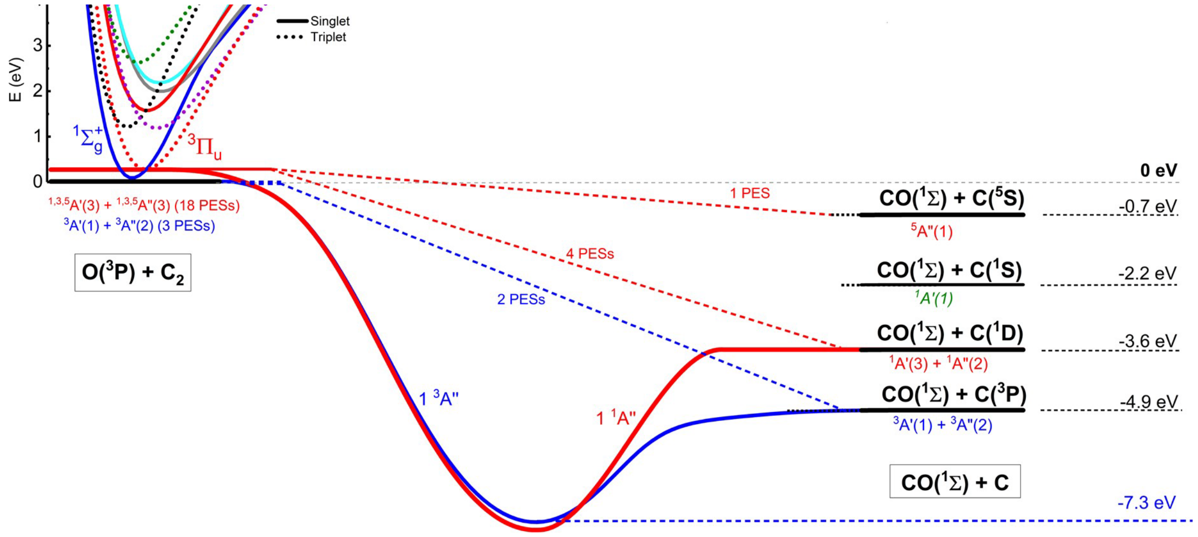

**Figure 1**. Correlation diagram for the O+C$_2$ reaction. In the left side, the entrance valley, and the lowest electronic states of C$_2$. The minimum energy path connecting the reactants and products on the 1$^1A''$ and 1 $^3A''$ PESs is also shown.

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# Theoretical study of ion-ion collision in iodine plasma for spacecraft propulsion

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Spacecraft electric propulsion provides a low thrust for a long period of time, which is particularly useful for interplanetary missions or for satellites trajectory correction maneuvers [1]. Recently, a new type of electric thruster was developed using iodine as a propellant. An iodine plasma is formed and an electric field expels ions from the reactor thus creating a thrust. The iodine has the advantages over other types of propellant (like Xenon) of being easy to store in a solid form and to be cheaper. The first launch of a satellite using iodine plasma took place recently (on November 6, 2020) with a thruster developed by the French start-up ThrustMe on a satellite of the Chinese aerospace company SpaceTy.

The development of more efficient iodine thruster is impeded by the lack of knowledge about the chemical properties of the iodine plasma [2]. In this work, our objective is to compute the cross-sections of the most important chemical reactions occurring in the plasma, in order to use them in a global kinetic model describing the plasma. In order to compute these cross-sections, we are using advanced relativistic electronic structure calculation [3] to obtain the relevant potential energy surfaces, and then a semi-classical dynamic method (i.e. Landau-Zener surface hoping [4]). I will present our first results concerning the neutralization reaction $I^+ + I^- \rightarrow 2I$. This is a particularly important reaction since it reduces the amount of ions in the plasma and thus lowers the number of species that could be used for propulsion. These results are in accordance with experimental measurements that were carried out in the ion ring DESIREE in Stockholm.

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# Electronic spectroscopy of $H_2O@C_{60}^+$ and $D_2O@C_{60}^+$

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Low temperature gas phase electronic spectra of $H_2O@C_{60}^+$ and $D_2O@C_{60}^+$ are presented. These data were obtained by one-photon dissociation of weakly bound helium complexes synthesised in a 3 K ion trap. The spectra of these endohedral fullerene cations are compared with the $A\ {}^2E_{1g} \leftarrow X\ {}^2A_{1u}$ electronic transition of $C_{60}^+$, and are found to be much richer in structure than the empty $C_{60}^+$, due to the excitation of (frustrated) rotations and/or vibrations of the encapsulated molecule. Results from two-colour experiments that allowed separation of *ortho* and *para*- $H_2O$ / $D_2O$ nuclear spin isomers stored in the trap are also presented and discussed.

# Data-driven approaches for modelling non-aqueous electrolytes

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Emerging machine learning technologies possess great potential to accelerate simulations for battery materials with atomic resolution. So far, such methods have been successfully employed to model small molecules in vacuum where the highly directional bonding interactions dominate and inorganic solids and liquids where the interactions are weaker but homogeneous. However, when it comes to addressing the complex chemical environments found in commercial battery electrolytes, it is essential to account for the large dimensionality imbalances between intra- and intermolecular interactions. Typical loss functions minimise total energies and forces in such molecular condensates, and since inter-molecular interactions are significantly weaker, ML models get good intra- and poor inter- relative accuracy. The most common strategy to overcome this problem is separating the interaction scales by creating independent force fields for the molecule and the liquid. This approach solves the problem of scale separation neatly; however, it also makes the extension of the model to the reactive regime a non-trivial task. In this work, we demonstrate that by crafting a sufficiently diverse training set through iterative training and carefully testing our models' accuracy on the relevant inter-molecular scale, we can fit a general-purpose potential that accurately describes the case of a solvent mixture commonly used in electrolytes for lithium-ion batteries. Thus paving the way for a more general and fully reactive force field, making it possible to model chemical reactions at the electrolyte-electrode interface/interphases with ab initio accuracy.

# Insights in the structure of homogeneous and hydrated Uracil clusters

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X-ray photoemission spectroscopy, XPS, is a very suited tool to probe the chemical environment of a specific atom in a system. In this work XPS has been used to study the different molecular interactions (H-bond, π-stacking, dispersion interactions) at work in homogeneous and hydrated uracil (U) clusters in the gas phase. The measurements have been performed at the Pleiades beam line [1] of SOLEIL synchrotron using a gas aggregation source, developed at CNRS-CIMAP [2] and coupled to an end station equipped with a Scienta R4000 photoelectron spectrometer. The measured C, N and O 1s XPS spectra of the clusters display a shift with respect to isolated uracil molecules [3] due to the variation of the molecular connections in the clusters. DFT-based simulations to calculate the binding energy of each atom in the cluster and molecular dynamics simulations to determine the cluster structure have been performed. The strategy of the simulation [4,5] is based on a bottom-up approach that selects aggregates with increasing numbers of uracil (2-50) and water (0-60) molecules to disentangle the effects of the different interactions in the cluster. In the case of the homogeneous clusters it was found that the formation of large clusters is driven by the anisotropic distribution of H-bond donor and acceptor sites, which can be also modulated by weaker dispersion forces [4]. In the mixed clusters the presence of hydrophobic moieties lead to the formation of a core-shell-like supramolecular organization in clusters of increasing size, where water forms tightly packed cores and uracil forms a shell around these cores [5].

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# Energy landscapes: from molecules and nanodevices to machine learning

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The potential energy landscape provides a conceptual and computational framework for investigating structure, dynamics and thermodynamics in atomic and molecular science. This talk will summarise new approaches for global optimisation, quantum dynamics, the thermodynamic properties of systems exhibiting broken ergodicity, and rare event dynamics. Applications will be presented that range from prediction and analysis of high-resolution spectra, to coarse-grained models and design principles for self-assembly of mesoscopic structures, with recent results for machine learning landscapes.

**Selected Publications:**

Ann. Rev. Phys. Chem., 69, 401-425, (2017). Exploring Energy Landscapes
Chem. Commun, 53, 6974-6988 (2017). Exploring biomolecular energy landscapes
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# Ultrafast dynamics of isomer-selected molecules

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Many gas-phase molecules possess isomers with distinct photochemistry, yet there are limited examples of cleanly selecting a given isomer and probing the excited state dynamics leading to isomeric products. This talk will describe some of our efforts to deploy multifaceted gas-phase experiments to investigate the excited state dynamics of anionic $E \rightarrow Z$ photoisomerising systems possessing barriers on the excited state to reaching an isomerising conical intersection seam. Action spectra and branching ratios associated with prompt photoisomerisation ($E \rightarrow Z$ and $Z \rightarrow E$) and electron loss are characterised using photoisomerisation action spectroscopy, a technique whereby molecules are separated according to their shapes before and after laser irradiation. Excited state lifetimes and the dynamics associated with electron detachment channels are characterised using frequency-, angle-, and time-resolved photoelectron imaging. For one system, time-resolved photoelectron measurements applying a series of pump photon energies find clear trends in excited state lifetimes and electron kinetic energy distributions associated a competition between internal conversion followed by autodetachment from a non-valence state and internal conversion to recover the ground electronic state followed by statistical electron ejection. Together, the experimental strategies provide a powerful and self-consistent means to deduce barrier-controlled excited state dynamics.

# Molecular photoionization in the weak- and strong-field regimes studied by the ab initio R-matrix method

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In this contribution I will describe our recent calculations studying the role of electron correlation in photon-induced processes in molecules. Addressing this topic in molecules is particularly difficult due to their lower symmetry, the need to describe accurately the wavefunction of the unbound electron and to consider the influence of nuclear dynamics. While inclusion of coupled electron-nuclear dynamics remains a challenge, our recent progress in development of the fixed-nuclei ab initio R-matrix method (UKRmol+) [1] and its time-dependent version (RMT) [2] has enabled accurate calculations of electronic dynamics of various photon-induced processes.

Our calculations of tunnel ionization of water [3] have shown that field-free and field-assisted inelastic scattering of the photoelectron has to be included to obtain even qualitatively correct results. The importance of electron correlation is found to vary with intensity of the driving field (10-1000 TW/cm$^2$), being most important at the lower intensities but still non-negligible at the higher intensities. A transition from below-threshold to above-threshold ionization is observed too.

In the perturbative regime we have calculated attosecond 2-photon RABBIT delays in $H_2$, $N_2$, $CO_2$, $H_2O$ and $N_2O$ [4] using our recently developed approach for direct evaluation of 2-photon molecular matrix elements. We have found an excellent agreement with $N_2$ and $CO_2$ but a poor one with $H_2O$ and $N_2O$ which is surprising in view of the excellent agreement of our 1-photon data with experiments. Crucially, we have uncovered a hitherto unrecognized contribution to RABBIT delays originating in field-induced near-resonant transitions in the ion. Our method allows, for the first time, to perform highly efficient and accurate calculations of the delays without the usually employed approximations, such as the separation of the RABBIT delay into the Wigner-Smith and laser-induced ones. This is only possible when correlation between the field-driven photoelectron and the residual ion is negligible. We confirm that this approximation is molecule-specific and that it may be inaccurate even at photon energies as high as approx. 40 eV.

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# Studying the competition between anionic and neutral excited state pathways in aromatic anions

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Photoexcited deprotonated anions can dissipate energy via several competing mechanisms. Fragmentation of the anion gives rise to anionic and neutral fragments, while photodissociation of the electron forms a dehydrogenated neutral radical which may be stable or may itself break up into neutral fragments. Depending on the relaxation mechanism(s) activated, the temporal profile of the observed neutral photoproducts will vary, as illustrated for a few examples in Fig. 1.

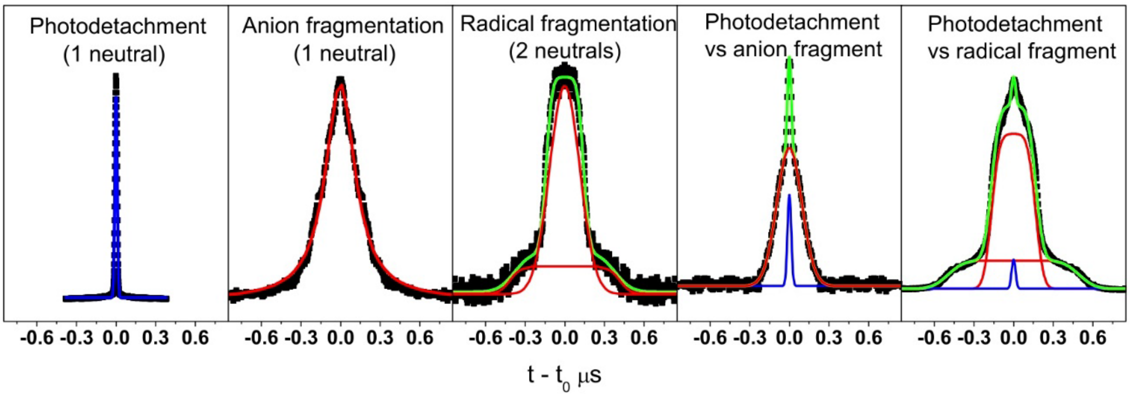

*Fig. 1: Observed temporal profiles of neutral photoproducts for varying relaxation mechanisms*

The study of the UV-visible spectra of a multitude of cold, isolated deprotonated aromatic anions – with varying functional groups and heteroatoms – over the past few years [1-5] has allowed our group to derive some general conclusions concerning the photostability of deprotonated aromatic anions and the structure and stability of their neutral photoproduct, the dehydrogenated radical.

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# Light matter interactions in dna origami assembled plasmonic nanostructures for single molecule spectroscopic study

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One of the promising applications that the DNA origami assembled plasmonic nanostructure finds its utility is in the field of single molecule surface enhanced Raman spectroscopy (SERS) study. Detection and study of molecular properties (especially of dyes, proteins or biomolecules) is of utmost importance before they could be employed for their potential utility. However, study of molecular properties at single molecular level using the principle of SERS demands precise positioning of the molecule at plasmonic hot-spot which shows maximum field enhancement for highest Raman signal.[1] Several strategies have been developed so far to create plasmonic nanostructures for precisely locating molecules at the hot-spot for single molecule studies using the principle of SERS.[2]

We propose a DNA origami technique to generate higher order DNA nanostructures for assembling plasmonic nanoparticles (in terms of plasmonic dimers) for precise positioning of molecules (biomolecules) at the hot-spot.[3] A tuning fork shaped DNA origami platform is designed to couple plasmonic particles with controlled gap distance following basic DNA hybridization. The uniquely addressable DNA sequence in the DNA origami design allowed positioning of dyes and biomolecule of interest at the hot-spot of assembled plasmonic nanostructures (dimers of Au and Ag). The high field enhancement at the plasmonic hot-spot with proper choice of laser wavelength allowed us to record SERS spectra of single molecule placed at the hot-spot of the dimer. The success of the SERS measurement of single biomolecule placed at the hot-spot of as-designed DNA origami based plasmonic nanostructures further opened up the possibility of studying external stimuli driven changes in molecular state of the biomolecule in single molecule scale.

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# Light-driven reactions in DNA

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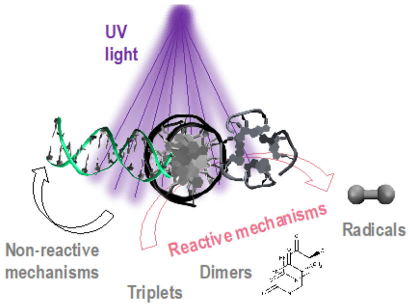
Nucleobases are the building-blocks of our DNA and absorb part of the UV radiation reaching the earth. This UV/DNA interaction originates a series of electronic excited singlet states whose characterization and evolution have been widely studied from the theoretical and experimental sides. [1,2] Most of them rapidly disappear preserving the structure of DNA and conferring its well-known photostability. Contrary, although minor for canonical structures, alternative reactive mechanisms can occur: as the creation of bonds leading to photodimers [3] connected with skin cancer or the generation of radicals [4] potentially increasing oxidative damage.

In the last years we have studied these excited states and their temporal evolution in canonical DNA, [5] chemical derivatives [6] and complex secondary structures (guanine-quadruplexes) [7]. We aim to fully understand these mechanisms at the molecular level what is important for, on one hand, the study of UV-induced DNA-damage and, on the other, the development of suitable fluorescent base analogs and/or the characterization of DNA/protein interaction.



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# The stability of defective PAH and fullerene ions over long timescales

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Using the cryogenic Double ElectroStatic Ion Ring ExpEriment (DESIREE) [1], we have studied how Polycyclic Aromatic Hydrocarbon (PAH) and fullerene ions stabilize after having lost individual carbon atoms in energetic collisions with helium atoms [2]. This process leading to the prompt loss of individual atoms, known as knockout, dominates when atoms and molecules collide at velocities around 100 km/s [3], a typical velocity of stellar winds and gas heated by shockwaves in space where these molecules are often found [2]. The knockout process is rather violent, but the products that are formed are generally more chemically reactive than their intact counterparts. This increased reactivity means that the fragments produced by knockout may play an important role in the chemical reaction pathways of astronomical environments where they are present. In our experiments we found that fragments of coronene ($C_{24}H_{12}^{+}$) and fullerene ($C_{60}^{-}$) ions that have had a C atom knocked out readily stabilize on millisecond timescales and that a large fraction of the fragments formed in this way are stable on astronomical timescales in the gas phase [2].

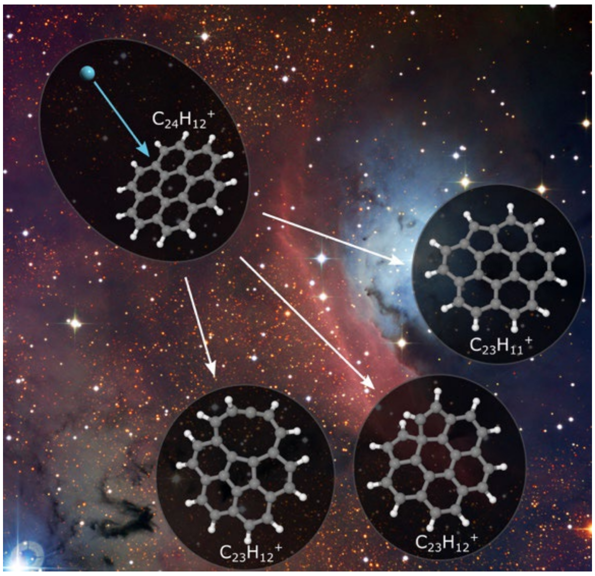

Figure: Examples of fragments formed when a C atom is knocked out of a coronene cation [2].

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# POSTER SESSION

# Control of ultra-cold molecular gases by optical shielding

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Ultracold polar quantum gases are promising systems with possible applications in quantum simulation or quantum computation. Due to their large permanent electric dipole moment polar molecules in electric field exhibit strong long-range anisotropic dipole-dipole interactions (DDIs). Nowadays, the creation and trapping of ultracold dipolar diatomic molecules of various species are feasible in many experimental groups. However long time trapping is still a challenge even in the case of the so called non reactive molecules [1]. To overcome the loss, we propose to suppress inelastic collisions using optical shielding (OS).

OS relies on the modification of long-range interactions between ground-state and excited molecules by laser light. The first experimental proof of the OS process was demonstrated in case of the collision between identical ultracold alkali-metal atoms [2]. One of the polar bi-alkali molecule for which unexpected losses were reported experimentally is the bosonic $^{23}$Na$^{87}$Rb molecule [3].

We will present our theoretical results on the OS of ultracold collision between two bosonic $^{23}$Na$^{87}$Rb molecule in their lowest rovibrational level of the ground electronic state. By applying a laser with a frequency detuned to the blue from the transition between the lowest rovibrational level of the electronic ground state $X^1\Sigma^+(v_X = 0, j_X = 0)$, and the long-lived excited level b $^3\Pi_0(v_b = 0, j_b = 1)$, the long-range DDI between the colliding molecules can be engineered. We have used a quantum close coupling method in the dressed-state framework to describe the two-body collision between ground state molecules in the presence of the OS field . The long range potential energy curves (PEC) between the two ground state molecule and between one ground state molecule and one excited molecule have been determined using a long-large multipolar expression [4]. Among a bunch of PECs, those with long-range repulsive behavior were identified as they are the best candidates for an efficient OS. We have carefully analyzed the ratio between the elastic and destructive (reactive and photoinduced inelastic) collisional rate ratio as a function of Rabi frequency and detuning to map the conditions for maximizing this ratio, which leads to efficient OS. Our calculations show that the proposed OS leads to a dramatic suppression of reactive and photoinduced inelastic collisions, for both linear and circular laser polarizations. We demonstrate that the spontaneous emission from b $^3\Pi_0(v_b = 0, j_b = 1)$ does not deteriorate the shielding process. This opens the possibility for a strong increase of the lifetime of ultracold molecule traps and for an efficient evaporative cooling. We also predict that OS is an effective mechanism for other heteronuclear alkali-metal diatoms with sufficiently large permanent dipole moment [5].

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# Thionitroxyl Radical (H2NS) Isomers: Structures, vibrational spectroscopy, electronic states and photochemistry

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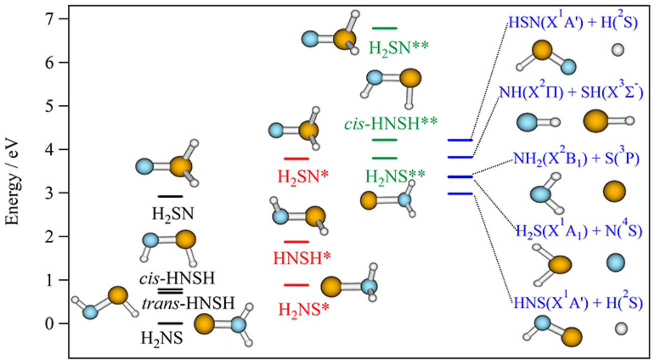
The thionitroxyl radical (H2NS) isomers are characterized using advanced ab initio methodologies. Computations are done using standard and explicitly correlated coupled cluster (RCCSD(T)) , CASSCF and MRCI approaches in conjunction with large basis sets, extrapolated to the complete basis set (CBS) limit. The lowest electronic states of different isomers are mapped along the stretching coordinates, thereby confirming the existence of the four already known ground state structures, namely H2NS, H2SN, cis-HNSH and trans-HNSH. Also, it is shown that only the lowest electronic excited states are stable, whereas the upper electronic states may undergo unimolecular decomposition processes forming H + HNS/HSN or the HN + SH or N + H2S or S + NH2 fragments. These data allow an assignment of the deep blue glow observed after reactions between "active nitrogen" and H2S at the beginning of the XXth century. For stable species, a set of accurate structural and spectroscopic parameters are provided. Since small nitrogen-sulfur molecular species are of astrophysical relevance, this work may help for identifying the thionitroxyl radical isomers in astrophysical media and in the laboratory.



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# Computational studies on the aggregation behavior in aqueous solutions

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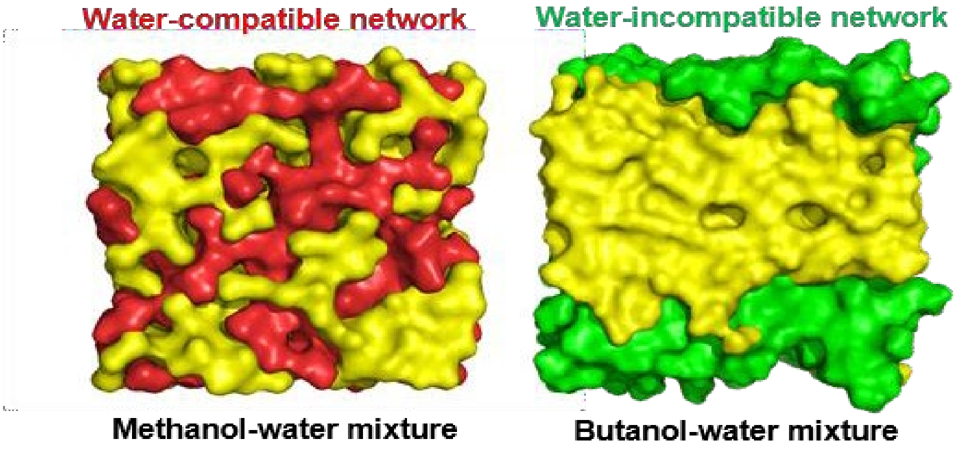
Water dissolves various molecules such ion, osmolyte, alcohol. As the concentration increases, the solute molecules are aggregated and the clustering behavior affects water H-bond network and further solution properties. Recently, we proposed a systematic theoretical approach by combining molecular dynamic simulation and graph theoretical treatment to analyze the solute aggregation behavior and water H-bond network properties. [1] Solute aggregation behavior was found to be classified into self- associating or network-forming in aqueous solutions which can be quantitatively described using graph theory. Interestingly, the self-associated solute molecules tend to separate from liquid phase, while the network-forming ones mix well with liquid water. That is, self-associated aggregation exhibits water-incompatible behavior and extended solute network is compatible with liquid water. This bifurcating aggregation hypothesis provides a reasonable clue as to how the solubility is affected by the nature of ions [1], the polarity of molecule [2], the shape of molecule [3], and the temperature [4]. Various computational studies in aqueous solutions were presented to examine quantitatively the solute aggregation and water H-bond network in use of molecular dynamics simulation and graph theoretical analysis.



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# Infrared spectroscopy of hydrated metal ions: A route to understanding the hydrogen evolution reaction

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Water activation at metal centres is paramount to the understanding of water splitting and formation of molecular hydrogen.[1-4] However, the exact mechanisms governing these processes are complex, thus model systems are required to understand the elementary steps and key intermediates during water activation. Gas-phase hydrated metal ions are ideally suited to serve as such models; molecular-level mechanistic steps can be probed in splendid isolation, without being obscured by counterions, aggregation, or other difficult-to-control effects.[5] The recent infrared spectroscopic studies on hydrated metal ions, which have been shown to act as key intermediates for the hydrogen evolution reaction, alongside reversible water activation, will be discussed.

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# Pickup and reactions of molecules on clusters: Solvent effects in generating the benzene radical anion

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Clusters of atoms and molecules have been investigated in molecular beams since the conception of the molecular beam technique. One of the motivations is to provide insight into the solvent effects in chemistry and physics at a molecular level. Our present research is inspired mainly by atmospheric chemistry (aerosols) [1] and astrochemistry (polyaromatic hydrocarbon nanoparticles) [2].

We have developed a versatile cluster beam apparatus CLUB in Prague to perform different experiments with clusters in molecular beams [3]. We will review some of our recent experiments, where different molecules are deposited on large clusters (nanoparticles) flying free in vacuum, and subsequent interactions with photons and/or electrons of different energies trigger processes such as UV-photodissociation, IR or UV excitation, ionization, electron attachment and ion-molecule reactions [3].

In particular, we will focus on our newest results involving benzene radical anion $C_6H_6^-$. It is an intriguing species, representing a stable anion in solutions, but it has the character of metastable shape resonance in the gas phase with a negative electron affinity EA = -1.15 eV [4]. Here we show the first evidence for a stable $C_6H_6^-$ ion in the gas phase. We generate large benzene clusters (of about 300 molecules) and an attachment of slow electrons (<10 eV) to these species yields a stable isolated $C_6H_6^-$ ion which survives at least 10-100 μs in our TOF mass spectrometr. This ion and its formation will be discussed in details.

Second, from the application point of view, the benzene radical anion represents an important intermediate in organic chemistry in the Birch reduction, where ammonia, benzene and solvated electron play a role [5]. To understand the underlying chemistry at a molecular level, we generate large ammonia clusters and dope them with single benzene molecules and subsequently attach slow electrons to them. Formation of solvated electron in ammonia and its subsequent localization on benzene generating solvent-stabilized $C_6H_6^-$ anion in ammonia are revealed and discussed.

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# Previously unidentified valence core-excited resonances in water

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The dissociative electron attachment (DEA) in gas-phase $H_2O$ proceeds via formation of three resonances located between 6.5 and 11 eV. The assignment of these resonances has been done in a classical work of Jungen et al. [1] via comparison with photoelectron spectra which reveal information about the grandparent cation states of resonances. $H_2O$ has a ground state electronic configuration of $[\ldots (b_2)^2 (a_1)^2 (b_1)^2]$. Jungen et al. assigned the three resonances to be of Feshbach type with an electron pair in a 3s Rydberg orbital and a hole in progressively lower orbitals, namely $(b_1)^1(3s)^2$, $(a_1)^1 3s^2$, $(b_2)^1 3s^2$. All the subsequent works on the DEA to water adopted this assignment.

We have recently constructed a DEA velocity map imaging spectrometer [2] which has several unique characteristics: (i) apart from VMI images, it yields absolute cross sections, (ii) it uses a monochromatized source of electrons and (iii) the compact dimensions of the ion optics system lead to small expansion of the Newton sphere of DEA fragments, such that the system has a good mass resolution. Specifically, in the $H_2O$ case we were able, for the first time, to separate the $O^-$ and $OH^-$ Newton spheres and record the corresponding velocity map images.

The experimental $O^-$ and $OH^-$ images are not consistent with the generally accepted assignment of resonances outlined above. First, if this assignment were valid, none of the resonant states could directly dissociate into the $OH^-$ fragment. In the past it has been speculated that this fragment has to come from ion-molecule reactions in the collision region. The present data clearly show that this is not the case. Second, the $O^-$ angular distributions do not agree with the theoretical distributions that assume the $3s^2$ resonant configuration.

Already in the early work of Spence [4] it has been pointed out that in a number of molecules also core excited-resonances with the electron pair in the 3s3p or $3p^2$ configurations are efficiently formed. The parent state (excited state of the neutral molecule) is often a triplet. In order to examine formation of such resonances we have measured the excitation efficiency of the four lowest triplet states of $H_2O$. The non-$3s^2$ resonances are clearly manifested in the excitation curves of these states.

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# Scattering Cross-Sections in Plasma Fluid Models

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Fluid models that accurately project the time evolution of low and high energy plasma systems are of high importance for the success of the International Thermonuclear Experimental Reactor (ITER) project. In order to develop such models, analytic models of collisional cross-sections must provide sufficient precision to capture the behaviour of plasma systems across a range of densities, projectile energies, temperature gradients and so on. As such, we seek to test the accuracy of commonly used scattering models in Monte-Carlo and Boltzmann-Solver programs, using a Monte-Carlo code developed by Reese Horton et al. in 2021 [1] which incorporates the highly accurate MCCC scattering cross-sections for electrons incident on H2 gas. The MCCC method employs the Born-Oppenheimer approximation to construct molecular electronic pseudostates in the Laguerre basis, which converge to the true states for sufficiently large basis size [2]. We present a comparative study comparing the accuracy of approximate cross-sections commonly used in MC models, such as those developed by Surendra et al. [3] and Park et al. [4], with the MCCC cross-sections for extraction of fluid transport parameters.

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# Hydration site controls dissociation dynamics of bromothiophenol anion

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Electron attachment to isolated and microhydrtated bromo- and nitro- thiophenols was investigated [1]. Thiophenols are common linkers between gold and complex organic molecules [2]. At the same time, when bound to nanoparticles, they can undergo rich surface plasmon mediated chemistry [3,4]. In our approach, isolated electron in vacuum interacts with microhydrated molecule, which imitate the mechanism of first electron reduction in the plasmon mediated chemistry [5].

We experimentally measured fragmentation spectra upon low energy (<8eV) electron attachment to isolated and microhydrated 4-bromo- and 4-nitro- thiophenol. Both molecules form stable parent anions or dissociate via the loss of electron affine Br or $NO_2$ groups, respectively. Upon hydration, parent anions are stabilized by the environment, however, in the case of bromothiophenol, also a series of hydrated fragment ions in the form $Br(H_2O)_n^-$ is observed. Quantum chemical modelling then shows that fragmentation and stabilization of the anion depends on the hydration site. Hydration on the Br site lowers the dissociation limit and allows for effective formation of hydrated fragments. Hydration on thiol site results in very stable parent anions. Fragmentation spectra after electron attachment, therefore, carry the information about hydration site of the neutral precursor and have a potential to become a tool to explore structure of small heterogeneous clusters.

This work was supported by Czech Science Foundation, project number 21-26601X (EXPRO).

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# Studying with DFT the electronic excitations of SOOT precursors

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Reducing soot emissions is of crucial importance according to the Intergovernmental Panel on Climate Change [1]. To do so, the scientific community is seeking to elucidate the soot's mechanism of formation and more specifically, to identify the molecular species responsible for the nucleation step. Polycyclic aromatic hydrocarbons (PAHs) are known to play a key role in the mechanism; [2] however, their precise role is still unclear. Using laser induced fluorescence (*in-situ*) it is observed that sooting flames display a broad fluorescence band in the visible region of the spectrum, which is suspected to be the fluorescence signature of nascent soot. [3] Interestingly, the fluorescence signals can be observed using low energy laser excitation in the visible range as well. In our work, we explore the optical properties of some PAH-based soot precursor candidates using DFT and TD-DFT. We focus more specifically on the effect of dimerization on the excitation spectra of small PAHs. We investigate the differences between chemically and physically bound dimers to look over their role in explaining the visible fluorescence band, and to confront it to the implication of other species such as radicals or trimers.

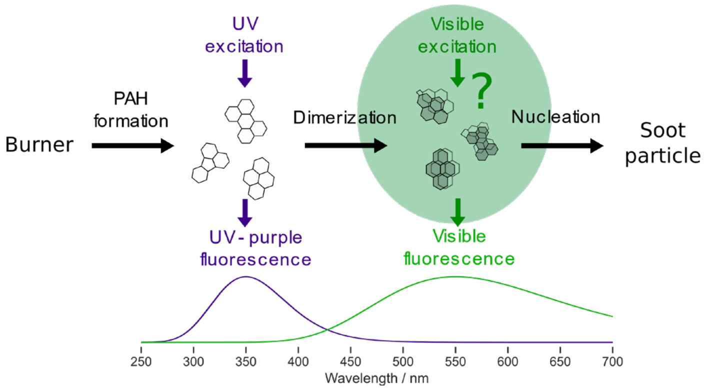

Figure: Depiction of the soot formation process in flames. The green area represents the topic of the presentation

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# Diatomic molecules of alkali-metal and alkaline-earth metal atoms: interaction potentials, dipole moments, and polarizabilities

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Ultracold diatomic molecules find application in quantum studies ranging from controlled chemistry and precision measurement physics to quantum many-body simulation and potentially quantum computing. Accurate knowledge of molecular properties is required to guide and explain ongoing experiments. Here, in an extensive and comparative study, we theoretically investigated the electronic properties of ground-state diatomic molecules composed of alkali-metal (Li, Na, K, Rb, Cs, Fr) and alkaline-earth-metal (Be, Mg, Ca, Sr, Ba, Ra) atoms. We studied 78 hetero- and homonuclear diatomic combinations, including 21 alkali-metal molecules in the $X^1\Sigma^+$ and $a^3\Sigma^+$ electronic states, 36 alkali-metal–alkaline-earth-metal molecules in the $X^2\Sigma^+$ electronic state, and 21 alkaline-earth-metal molecules in the $X^1\Sigma^+$ electronic state. We calculated potential energy curves, permanent electric dipole moments, and polarizabilities using the CCSD(T) and CCSDT coupled cluster methods with large Gaussian basis sets and small-core relativistic-energy-consistent pseudopotentials. We collected and analyzed corresponding spectroscopic constants. We reviewed previous experimental and theoretical data and compared them with the present values to establish a new benchmark. Presented results should be useful for further application of the studied molecules in modern ultracold physics and chemistry experiments.

# 2D Electronic spectroscopy of CdSe quantum dots pinpointing excitonic states, their size dependence and dynamics

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Colloidal quantum dots (QDs) have attracted interest as materials for opto-electronic applications. Their excitonic states form closely-spaced atomic-like bands that depend on QD size, causing e.g. heterogeneous spectral broadening. Efficient use of energy in QD devices requires detailed understanding of carrier relaxation and traps caused by functionalization of QDs. The high temporal and spectral resolution of 2D electronic spectroscopy (2DES) makes it an ideal tool for the study of exciton states and dynamics in QDs. Here, we provide an overview of our 2DES work on CdSe QDs with a broad size distribution, including relaxation and trapping [1,2], phonon beatings, and size effects on cross peaks and biexciton shifts. Our first analysis focused on states closest to the band edge, where we observed hole trapping into a size-independent state below the band edge. To further extend the covered set of states, we use two-color 2D spectroscopy. Together, single- and two-color 2D spectra at 77 K enable us to pinpoint well-defined bright states and dynamics that indicate the presence of weakly absorbing states providing a relaxation and trapping pathway around the phonon bottleneck [3]. From the slopes of cross peaks, we can obtain the size dependence of state energies in a much less time-consuming way than previous methods [4], as well as the biexciton shift at the band-edge state and its size dependence. By Fourier transforming the population time axis, we identify the size-independent oscillations in the 2D signal as longitudinal optical phonons. Together, these results showcase the versatility of information that can be extracted from a small set of 2DES measurements.

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# Actinide chemistry with pCCD-tailored CCSD

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The interactions between actinide atoms with surrounding atoms are a computational challenge as electronic structures of the actinide-containing molecules are highly afflicted by relativity and electron correlation effects. We elucidate the activation of the uranyl oxo bond in uranium-containing complexes [1] using relativistic Hamiltonian combined with the state-of-the-art correlated wave function models based on geminal theory and coupled-cluster theory [2]. Moreover, we use quantum information theory [3] to dissect the process of reducing the strong U–O interactions while preserving the weak nitride uranyl bond.

Strong electron correlation effects can be modeled using the tailored coupled-cluster approach. The subset of cluster amplitudes is extracted from the external model to provide the proper description of the multi-reference nature of the molecular system. Our work focuses on coupled-cluster models tailored by orbital-optimized pair coupled cluster doubles (pCCD) [4, 5]. These methods scale polynomially with the system size and provide a robust way to include strong electron correlation effects.

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# Molecular modelling of the influence of heparin/heparan-sulfate-derived oligosaccharides on human interferon gamma binding and dynamics

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Human interferon-gamma (hIFNγ) is a signaling molecule (cytokine), which plays a crucial modulating role in the initiation and development of immune response against various pathogens. To exert its pleiotropic effects on cells the protein binds with high affinity to a specific cellular receptor, the hIFNγR1. Experimentally, it is known that the cytokine also binds with high affinity to glycosaminoglycans (GAGs), in particular heparin and heparan sulfate (HS). This interaction affects significantly its physico-chemical properties.

We employed molecular dynamics (MD) simulations to model the interaction of hIFNγ and heparin/heparan-sulfate-derived oligosaccharides and to study the influence of this interaction on the formation of the cytokine-receptor complex. We found that the carbohydrate chains play a two-sided role in the binding of hIFNγ and hIFNγR1.

On the one hand, modeling the interaction of heparin and the free cytokine in the circulation provides evidence for the inhibitory effect of this GAG on the formation of the hIFNγ—hIFNγR1 complex. The oligosaccharides bind to the C-termini of free IFNγ with high affinity, forming very stable complexes due to the strong electrostatic attraction. However, they and also interact with the positively charged solvent-exposed domains in the cytokine globule. This impedes further interaction of the cytokine with hIFNγR1 and thus inhibits the complex formation.

On the other hand, GAGs, and HS in particular, may be crucial participants in the formation of the hIFNγ–hIFNγR complex at the cell surface. HS oligosaccharides are present ubiquitously at the cell membranes as part of the HS proteoglycans, covering almost all cellular surfaces. Our molecular modeling results demonstrate that placing HS oligosaccharides between the two receptor units facilitates the formation of the cytokine–receptor complex by pulling down the hIFNγ globule via electrostatic attraction of its C-termini. Experiments performed on cell cultures qualitatively confirm our molecular modeling results.

## Acknowledgments:

This work was supported in part by the Bulgarian National Science Fund under Grant DN-11/20/2017. Computational resources were provided by the Centre for Advanced Computing and Data Processing, supported under Grant BG05M2OP001-1.001-0003 by the Science and Education for Smart Growth Operational Program (2014-2020) and co-financed by the European Union through the European structural and investment funds.

# Excited-state mixing in light-Oxygen-voltage-sensing domain proteins studied by transient resonance Raman spectroscopy

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Flavin mononucleotide (FMN) is a biomolecule that functions as cofactor in many biochemical processes. In previous work, we applied transient absorption and femtosecond stimulated Raman spectroscopy (FSRS) to elucidate the photophysics of this chromophore. Time-resolved spectra were taken with time delays up to a few ns after FMN photoexcitation and the observed Raman bands in the excited singlet $S_1$ and triplet $T_1$ states were assigned with the help of quantum chemistry calculations.[1] Here, in order to understand the influence of the protein environment on the photophysics of FMN, we measured FSRS of FMN bound to EL222, a photosensory receptor containing a light-oxygen-voltage (LOV) domain. Moreover, we extended the timescale of our experiments up to 0.5 ms. Based on the experimental data we concluded The displacement amplitude between the excited-state potential energy surface (PES) minima that was estimated using the displaced harmonic oscillator model. We propose a change in the topography of the potential energy surface in the $S_1$ state due to protein-mediated mixing of the $\pi\pi^*$ state and the $n\pi^*$ state of FMN. The mixing is supported by the decrease of the corresponding transition dipole moment with a higher electronic state. We speculate that such a mixing may arise from non-symmetric hydrogen bonds between the $O_4$ atom of FMN and two surrounding amino acid residues in the EL222 binding pocket. The mixing might also be favored by a smaller energy gap between these two states due to the interactions between the FMN moiety and the LOV cage. In principle, the $n\pi^*$ feature of the $S_1$ state will decrease the electron density of the FMN $N_5$ atom and reduce its proton affinity.[2] This provides a perspective to understand the primary photochemical reaction in the LOV domain that occurs on the $T_1$ state rather than the $S_1$ state.

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# Electron Induced Reactivity of Methyl Methacrylate

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Polymethyl methacrylate is commonly used as a resist material for electron beam, UV and x-ray lithography. Secondary electrons are believed to play an important part in lithographic processes.[1] Furthermore, it has been shown that polymerization of methyl methacrylate (MMA) can be initiated by electron bombardment.[2] For these reasons, understanding the electron-induced reactivity of MMA is a topic of great importance.

Using the Troichoidal Electron Monochromator-Quadrupole Mass Spectrometer apparatus,[3] we investigated electron attachment (EA) to isolated MMA in the gas phase. In total, twelve anion products were observed for EA to MMA, with the most intense being $OCH_3^-$. Associative electron attachment to form the parent anion was not observed. For each product, the electron energy dependant ion yield was measured in the range 0-12 eV.

EA to MMA clusters was studied using the CLUster Beam apparatus.[4] EA to MMA clusters was found to produce a different distribution of anion products than to isolated MMA. Clusters of the parent ion were observed, up to $M_{11}^-$, with the intensity of the parent ion monomer ($M^-$) being much lower than expected and the dimer ($M_2^-$) being much higher than expected.

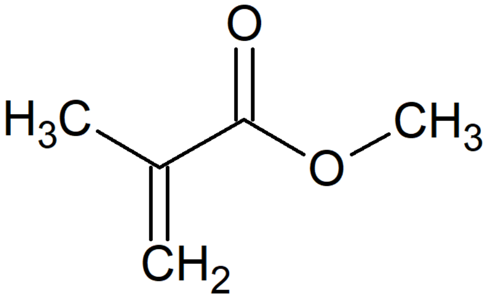

**Fig 1:** Chemical structure of methyl methacrylate.

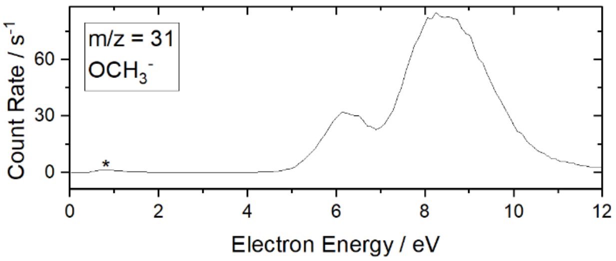

**Fig 2:** Electron energy dependance of $OCH_3^-$ for electron attachment to isolated methyl methacrylate.

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# Influence of magnetic field on Newton sphere of charged particles in imaging experiments

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In the velocity map imaging (VMI) experiments, a presence of the magnetic field which is perpendicular to the VMI spectrometer is sometimes necessary. This is especially the case in electron-impact experiments where such a field is used to guide the incident electron beam. The magnetic field necessarily influences the Newton sphere of ionic fragments and thus the shapes of the resulting images.

We have systematically studied this effect using particle trajectory simulations. A negatively charged oxygen ion was taken as an example. The simulation was performed in the Simion software package, where an exact virtual copy of an existing VMI setup was created with real values of the magnetic and electric fields. The generated initial parameters were set in Simion for each particle with a uniform distribution. As part of this work, the behavior of particles at a distance of 165 mm from the source position was tested with different values of the magnetic field as well as with different initial positions. The values of the particle's time of flight and its position in space were stored in the output files.

Using the Simion output files, the images with and without magnetic field were generated using Python scripts. These images were generated for short time intervals corresponding to time slices of the Newton sphere such that they are directly comparable with the experimental data which are taken using a time-and-position sensitive delay-line detector. These data thus enable us to identify experimental artifacts in the images which are due to the presence of the magnetic field.

# Mass spectrometry at the limits of biological objects: Viruses, bacteria and amyloid fibers

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Bioparticles consisting of self-organized biomolecular assemblies are ubiquitous in nature. Viruses are a good example of this and are the most abundant and robust biological entities on Earth.

New electrostatic traps (Benner trap) based on charged detection mass spectrometry (CDMS) have recently been set up to carry out fragmentation experiments on selected ions with masses up to several GigaDalton [1]. One of this setup has been developed in the SpectroBio group of iLM at University of Lyon 1, allow coupling with a laser and performing infrared multiphoton dissociation, monitoring fragmentation and determining the activation energy of unimolecular dissociation of bioparticles and whole DNAs [2,3,4].
A large part of this project will be to develop both an analytical chemistry approach to characterize bioparticles by mass spectrometry, and to push the limits of photo-fragmentation induced by laser irradiation on intact viruses or other bioparticles (bacteria or amyloid fibers) to develop new structural characterization tools.

This project is part of the FET-OPEN ARIADNE VIBE (Airborne Ion Analysis with Dissociation and Non-destructive Evaluation of Viruses and Bacteria – Grant agreement 964553) funded by Europe on the characterization of viruses and bacteria using CDMS technique.

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# Parametrization of reduced density matrices for quantum fluids: From unimolecular reactions to multi-adsorbate dynamics

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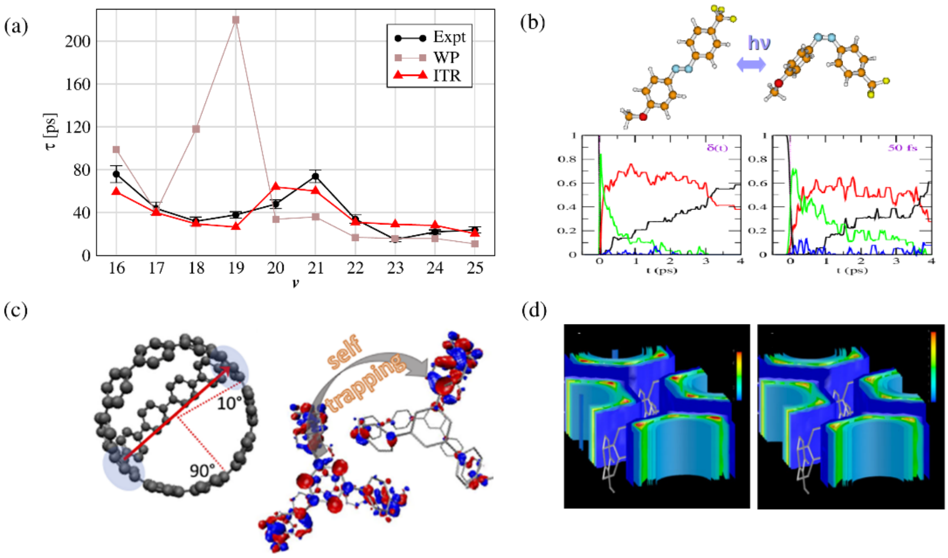
**Abstract**. Tailored representations of reduced density matrices for the electronic and the nuclear degrees of freedom are benchmarked on model systems (e.g., atomic photoelectron spectra, vibrational predissociation of van der Waals triatomic complexes), and subsequently applied to more challenging phenomena (e.g., adsorbate reaction dynamics, elementary excitations in doped helium droplets, interatomic coulombic decay in paired quantum dots, non-adiabatic photoisomerization of molecular switches, exciton dynamics in organic conjugated polymers). The density-matrix based simulations target nanoscale systems which constitute promising candidates for technological applications in hydrogen production and storage in nanomaterials, high-resolution spectroscopy, and optoelectronics. We assess the numerical convergence, accuracy and stability of the proposed algorithms for quantum molecular dynamics simulations. The computed observables exhibit a close correspondence with previous experimental and theoretical results for the target systems.



(a) Computed lifetimes of the predissociating $\mathrm{ArBr_2}(B,\nu)$ van der Waals complexes.

(b) Isomerization dynamics of an azobenzene derivative (TF-Az-OMe).

(c) Exciton self-trapping in carbon nanocages.

(d) Contour plots of the molecular hydrogen density inside the unit cell of (4,4) armchair carbon foams.

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# Study of the effect of higher-order dispersions on photoionisation induced by ultrafast laser pulses applying a classical theoretical method

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We investigated the effect of higher order dispersion on ultrafast photoionisation with Classical Trajectory Monte Carlo (CTMC) method for hydrogen and krypton atoms. In our calculations we used linearly polarised ultrashort 7 fs laser pulses, $6.5 \times 10^{14}$ W/cm$^2$ intensity, and a central wavelength of 800 nm. Our results show that electrons with the highest kinetic energies are obtained with transform limited (TL) pulses. The shaping of the pulses with negative second- third- or fourth- order dispersion results in higher ionisation yield and electron energies compared to pulses shaped with positive dispersion values. This phenomenon can be quantitatively characterised by the asymmetry parameter defined as

$$A(D) = \frac{N(D) - N(-D)}{N(D) + N(-D)}$$

where *N(D)* is the number of photoelectrons at a given value of dispersion. We have also investigated how the Carrier Envelope Phase (CEP) dependence of the ionisation is infuenced by dispersion. We calculated the left-right asymmetry defined as

$$A(E, \varphi_{CEP}) = \frac{N^+(E, \varphi_{CEP}) - N^-(E, \varphi_{CEP})}{N^+(E, \varphi_{CEP}) + N^-(E, \varphi_{CEP})}$$

where $N^+$ and $N^-$ mean the number of electrons having positive and negative momentum along the polarization axis respectively. We carried out the calculations for sodium atoms employing pulses of 4.5 fs, 800 nm central wavelength, and $4 \times 10^{12}$ W/cm$^2$ intensity. We found that the left-right asymmetry is more pronounced for pulses shaped with positive Group Delay Dispersion (GDD).

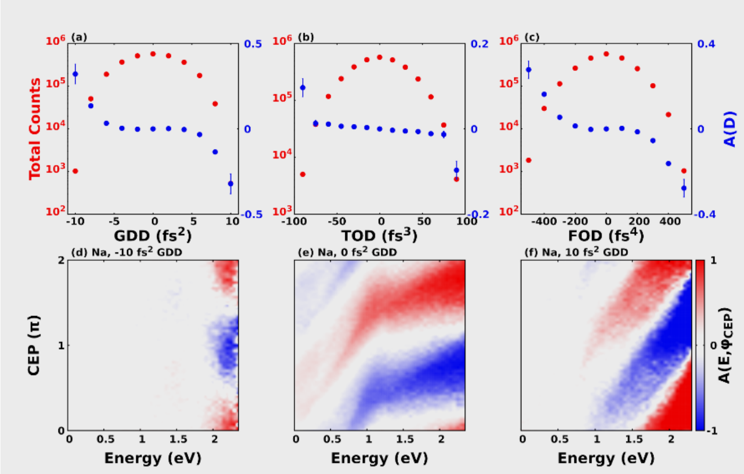

FIG. 1. Number of electron counts and asymmetry parameters for hydrogen calculated with different GDD (a), TOD (b) and FOD (c). Calculated maps of the asymmetry defined by Eq. (2) for Na at $4 \times 10^{12}$ W/cm$^2$ intensity with different values of GDD (d)-(f).

# Interpretation of shake-up mechanisms in copper L-shell photoelectron spectra

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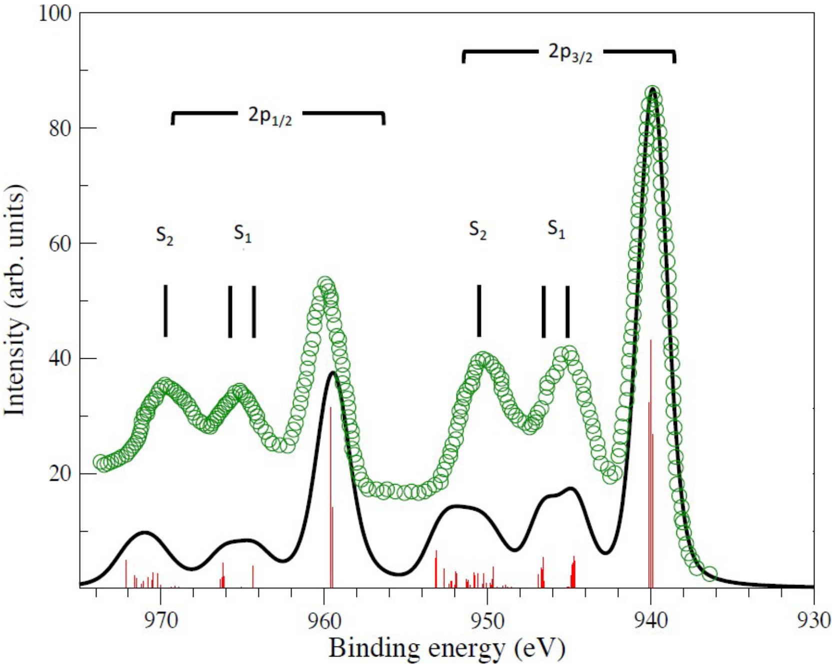
We report on an original and general approach enabling to elucidate the underlying mechanism structuring the CuL-shell photoelectron spectra through the revisited analysis of the Cu(acac)2 molecular compound. The creation of a 2p core-hole leads to an energy drop of the Cu3d levels which switches the nature of the Highest Singly Occupied Molecular Orbital (H-SOMO) from a dominant metal to a dominant ligand character. This gives rise to new bonding and anti-bonding orbitals and is accompanied by specific shake-up excitations (Ligand → Ligand and Metal → Ligand) towards the relaxed H-SOMO. The unambiguous identification of this characteristic relaxation mechanism sheds light onto the still debated nature of the main and satellite lines observed in the photoelectron spectra of 3d transition metal compounds.

The figure indicates the Cu2p theoretical photoelectron spectrum of the Cu(acac)2 molecule calculated within the CI b1g model. The black curve corresponds to a 2 eV width Voigt profile applied to the raw intensities (red bars). In comparison is shown the experimental spectrum recorded by Okada et al. [1] for the Cu(acac)2 molecule (green circles). Cu 2p3/2 and Cu 2p1/2 regions are indicated, as well as S1 and S2 satellite bands. As shown, the proposed ab-initio model enables us to reproduce the 2p XPS spectrum which is in good agreements with excremental data.



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# Theoretical Auger spectroscopy of aqueous solutions

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Auger-type spectroscopies have been recently recognized as a powerful tool for exploring relaxation processes after X-ray irradiation.[1] In my contribution, I will devote to K-edge Auger spectra interpretation for a series of solvated isoelectronic cations ($Na^+$, $Mg^{2+}$ and $Al^3$). Specifically, the non-local relaxation processes as Intermolecular Coulomb Decay (ICD) and Electron-Transfer Mediated Decay (ETMD) processes and their spectral manifestation will be shown and discussed in more detail. Both processes are dependent on the immediate "chemical environment" of the ionized metal ion and allow to directly "see" the binding strength of ions to the solvent and to identify speciation of ions. However, the theoretical interpretation of the measured data is highly non-trivial. I will point out the recent development in *ab initio* protocols for complicated electronic structure problems (during the relaxation, highly charged particles are created) and new approaches for solvent modelling (long-range polarization is crucial for correct energy estimate).

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# Halogen substitution effect on the photodissociation of acetyl chloride: A velocity map imaging study at different exciting wavelengths

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Photochemistry of acetyl chloride is important from both fundamental and environmental point of view as unlike usual Norrish type I reaction the stronger C-Cl bond is broken over a weaker C-C bond upon UV absorption and produce highly reactive Cl atom, harmful to the tropospheric atmosphere.[1] Here, we have investigated the effect of halogen substitution at β-carbon on photodissociation by velocity map imaging (VMI) of fragmented Cl by employing (2+1) REMPI at 235 nm. We have studied $CF_3COCl$, $CCl_3COCl$ and $ClCH_2COCl$ with different exciting wavelengths ranging from 193 to 280 nm. Though the translational energy distribution (TED) of Cl is similar for fluorene substituent and parent $CH_3COCl$, an indication of direct dissociation, the Cl substitution showed more complex mechanisms with possible multiple channels. Even for $CF_3COCl$, the TED of Cl and Cl* exhibit different behaviour at the lower translational energy region while exciting at 193 nm (Figure 1). We have also investigated the fragmentation channel producing CO as in our experimental UV energy range the single-photon energy is sufficient to induce different pathways.

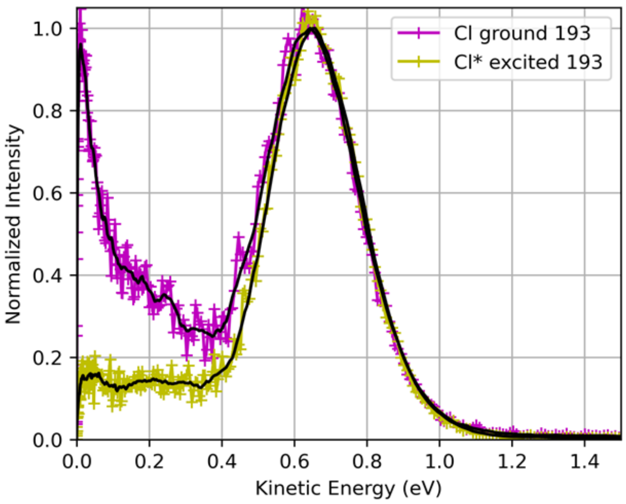

Figure 1 The TED of Cl and Cl* after photodissociation of $CF_3COCl$ at 193 nm

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# Setup for electron beam-induced chemical reactivity in liquid phase

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We present a recently developed experimental setup to be used to study electron beam induced reactions with molecules solvated in the liquid phase. One of the motivations 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. The experimental results will also enable us to understand the effect of liquid environment in the event of electron beam induced reactions.

The experimental setup is equipped with a high-vacuum compatible liquid micro-jet source and an electron gun producing an electron beam with tuneable energy in between 100 to 1000 eV. The liquid jet is produced by flowing the liquid, with 0.7 to 0.9 ml/min flow rate, through a small quartz nozzle with either 30- or 50-micron inner diameter using an HPLC pump producing around 50 to 120 bar pressure. Around 3 mm long liquid beam is exposed inside the high vacuum (of $10^{-5}$ mbar range) and then collected back either for recycling or for further analysis.

The chemical changes in liquid samples are analysed offline using standard analytical techniques such as UV-VIS spectroscopy or gel electrophoresis. Some initial results on the electron-beam induced reactivity in aqueous solvated TRIS (2-Amino-2-(hydroxymethyl)propane-1,3-diol) will be presented.

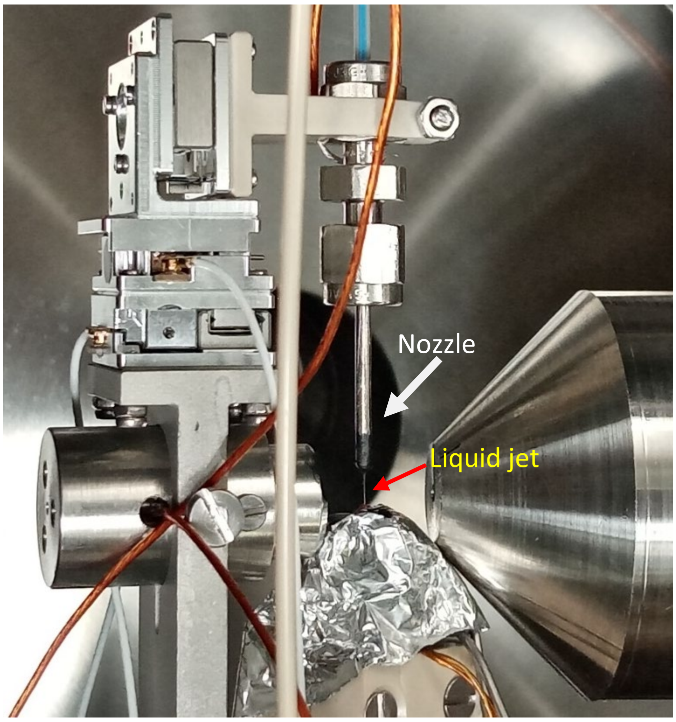

Fig.1, Picture of the liquid micro-jet setup showing the nozzle, running liquid jet, Faraday cup and part of the electron gun and liquid re-circulating system are shown.

**Acknowledgments:** This work was supported by Czech Science Foundation, project number 21-26601X (EXPRO).

# Superglass state in an optically realizable model

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A superglass phase was first experimentally observed in solid $^4$He [1] and initially identified as a supersolid [2]. The uniqueness of this phase comes from the fact that it requires two competing orders, superfluidity and glassiness, to coexist. Physical systems where this competition can be observed and studied in a controllable way are scarce. However, the development of quantum simulation techniques, e.g., using ultracold atoms in optical lattices, paves the way toward experimental studies of such systems. Combining a theoretical study of a model Hamiltonian with such a simulation will allow for determining the roles of system components and a better understanding of the superglass state.

In this contribution, we theoretically study a system of strongly correlated disordered bosons, which can be simulated using an optical lattice [3, 4]. We find that this system features a superglass phase in addition to disordered, glassy, and superfluid ones.

We model the system using the Bose-Hubbard Hamiltonian with gaussian-distributed random tunneling terms. We employ the replica trick and Trotter-Suzuki expansion to arrive at a set of self-consistent equations, which we then solve numerically. Using their solution, we evaluate critical line conditions [5] to find the phase diagrams of the system. We calculate the latter for various choices of system parameters. Additionally, we characterize the phases based on the values of the order parameters, compressibility, and behavior of dynamical correlations [6].

Finally, we suggest a feasible way [3] to simulate the studied model using an array of elongated ion traps in a woodpile arrangement. There, the two layers of traps are perpendicular to each other and coupled via Josephson junctions. The tunneling disorder is realized by randomizing the distances between the traps.

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# Gas phase generation of reactive species and investigation them in clusters

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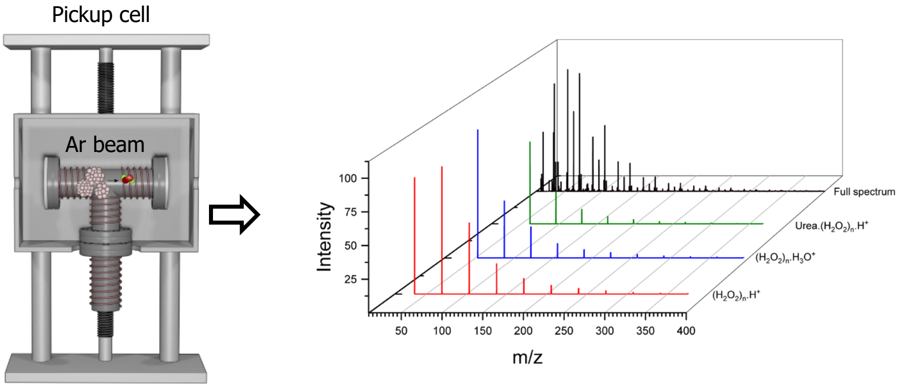
Short-lived species such as radicals drive many chemical reactions in different environments. The gas phase studies of the radical chemistry allow to limit their reactivity and thus provides necessary information of their structure and dynamics however relevant only for bimolecular systems. Here we present new research approaches for studies of variations in the gas-phase dynamics of the reactive species due to cluster environment and thus revealing the aspects of interfacial chemistry. We investigated electron induces chemistry of hydrogen peroxide, $H_2O_2$, when it was deposited on the argon or water clusters, $Ar_N$ /$H_2O_N$, respectively. Reactivity of Cl containing radicals with methane residing on $Ar_N$ surfaces was also studied. To produce a clean source of $H_2O_2$ the special setup for gentle evaporation of $H_2O_2$ from the stable complex of urea with hydrogen peroxide (UHP) was built and introduced into the clusters beam apparatus (CLUB). The beam of chlorine radicals was generated using the home-built source for pyrolytic decomposition of the $CCl_4$ precursor diluted in He rare gas. The argon clusters composed of up to 200 atoms showed to be a suitable environment for the deposited species to meet each other, make complexes or react with each other. The mobility of the hydrogen peroxide molecules on the water clusters showed to be restricted by the preferential formation of the water-hydrogen peroxide bonds rather when formation of $H_2O_2$ dimers. The electron attachment experiments with $H_2O_2$ deposited on $Ar_N$ provided insight into the possible intra-cluster reactions in the formed $(H_2O_2)_M$ complexes. The studies of the reactions of products of $CCl_4$ pyrolysis with methane on $Ar_N$ supported the previous conclusions that reactivity on the argon surface is facilitated by much higher ability of the molecules to meet and thus to react.



# Resonances in nitrobenzene probed by the electron attachment to neutral and by the photodetachment from anion

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In this work we investigate resonances in nitrobenzene by probing the transient anions and observing the subsequent electron emission from them. Experimentally, the resonances are populated in two ways - by electron impact of free neutral molecules by means of 2D electron energy loss (EEL) spectroscopy [1], and by photo-induced excitation of molecular bound anions using 2D anion photoelectron (PE) spectroscopy [2]. The two methods lead to an excitation of anion which is in different initial geometries, which results in differing electron emission mainly seen in excitation of vibrational modes, however some common features are observed as well.The obtained electron spectra from the two experiments show several types of emission. Those are two basic types - specific vibrational excitation and unspecific vibrational excitation which leads to emission of thermal electrons. Moreover, we observe a third type - involving a nonvalence dipole-bound state of anion [3, 4], which is characterized by an emission of very slow electrons but with a structure resembling specific excitation. Depending on how the resulting molecule is vibrationally excited, the electron spectra are showing that a very different specific vibrational modes are excited by electron collision and photodetachment, due to dependence on initial anion geometry. For the case of electron collision experiment that is of a neutral molecule, while for photodetachment experiment anions are prepared by molecular beam source and have a slightly longer $NO_2$ bond length. Electron energy loss spectra are dominated by out of plane bending modes, CN stretch and $NO_2$ asymmetric stretch modes, while photodetachment spectra show mainly $NO_2$ symmetric stretch modes and its overtones. On the other hand, unspecific vibrational excitation proceeds with internal vibrational redistribution, where both experiments show similar emission of thermal electrons from hot ground anion state. A model based on detail balance principle for the statistical electron emission is in a good agreement with this experimental observation. Furthermore, the third type of electron emission identified as vibrational autodetachment featuring electrons emitted with a fixed energies for a very broad range of excitation energies is similar in both experiments. In this work we examine the entrance channels for such vibrational autodetachment in detail, where our results suggest a new mechanism that involves a reverse valence to non-valence internal conversion.

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# Multiply Charged Superfluid Helium Droplets

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Superfluid helium nanodroplets (HNDs) [1] have been widely used as a cryogenic matrix in studies of complexes such as gold clusters [2]. To provide better insight into the nature of HNDs and their interaction with embedded dopants, the influence of electron impact ionisation on pristine superfluid helium nanodroplets has been investigated. HNDs with a uniform velocity distribution and containing up to several billion atoms are produced via supersonic jet expansion. This study utilizes a tandem setup consisting of an electron impact ion source and electrostatic ioniser, followed by a second identical ioniser and analyser. The two-staged setup allows for a selection of the droplets after the first ionisation source depending on their mass-to-charge ratio and additional probing through the second ioniser.

Depending on polarity, ionisation parameters and droplet size, the resulting mass to charge distribution of the product droplets varies greatly. Multiply charging of selected droplets can be observed for cationic as well as for anionic droplets. We could identify anionic helium droplets carrying up to five charges and cations exceeding 50+ charge centres [3,4]. The appearance sizes for multiply charged anions are found to be two orders of magnitude larger than for the corresponding cationic droplets [3,4].

This work is supported by the Austrian Science Fund, FWF via project numbers W1259-N27 and I4130.

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# DNA origami nanoframes as platforms to investigate DNA radiosensitization by halogenated nucleosides

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Understanding the underlying mechanisms of DNA damage upon exposure to ionizing radiation and in the presence of radiosensitizing agents is crucial in the improvement of radiation therapy against cancer [1]. Molecules sensitive to low energy electrons in the gas phase have been predicted to have radiosensitizing properties and evaluating their damage enhancements to DNA in solution is beneficial before moving to *in vivo* and eventually, clinical applications. The use of DNA origami nanosubstrates presents a promising approach to test radiosensitizing agents particularly, halogenated nucleosides such as 8-bromoadenosine (BrA) and 2’-deoxy-2’-fluorocytidine (2FC). Formed from folding single-stranded DNA scaffolds using short complementary strands (staples), rigid 2D origami nanostructures can be assembled on which one can attach molecules of interest at addressable sites [2]. DNA origami nanoframes (Fig. 1) containing an inner aperture to support DNA sequences of interest and sensitizing nucleosides are irradiated with high energy electrons (16 MeV) revealing different radiosensitizing mechanisms including “bystander effects” to nearby unsensitized strands as evidenced by total lesion yields derived from real-time polymerase chain reaction (RT-PCR) data and double-strand break yields (DSB) observed in atomic force microscopy (AFM) images of irradiated samples [3]. BrA shows enhancement to both total lesions and DSB while 2FC shows only enhancement in DSB at the same number of total lesions and both affect the strand break yields of the parallel unsensitized control strand situated ~10-12 nm away showing long-range diffusion of formed reactive radiolysis products. This work illustrates the potential of such nanosupports as tools in observing mechanisms of DNA damage and radiosensitization in conditions close to intracellular environments.

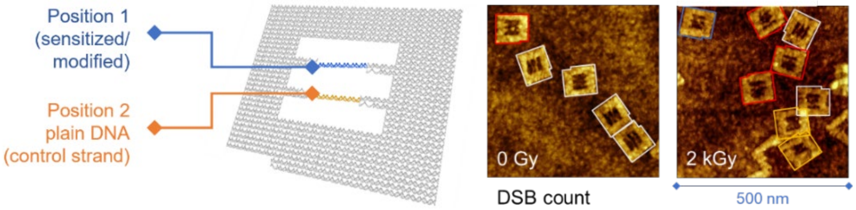

Figure 1. Scheme of the DNA origami nanoframes and AFM images of unirradiated and 16 MeV electron-irradiated samples, with a total absorbed dose of 2 kGy.

**Acknowledgements:** Praemium Academiae, and projects “Center for Tumor Ecology - Research of the Cancer Microenvironment Supporting Cancer Growth and Spread” (Reg. No. CZ.02.1.01/0.0/0.0/16_019/0000785) and CARAT (Reg. No. CZ.02.1.01/0.0/0.0/16_026/0008382) supported by the Operational Programme Research, Development and Education.

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# A Molecular Dynamics simulation insight into the Histidine Tautomeric effect on early stages of diabetes Mellitus progression and cross-seeding of $A\beta_{40}$ and hIAPP$_{1-37}$

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In 2021, around 537 million people around the world have been affected by Type 2 diabetes (T2D) which has been projected to rise to approximately 783 million by 2045. As it is known, Amyloid-β (Aβ) and human islet amyloid polypeptide are the main pathological species in Alzheimer's disease AD and T2D, respectively. Meanwhile, some clinical studies have indicated a possible risk factor and connection between T2D and AD formation. Although the early stage aggregation of amylin and co-aggregation mechanisms of these two amyloidogenic peptides is still largely unknown. Herein, For the first time, we elucidated the influence of histidine tautomerism on the aggregation of amylin and cross-seeding between human islet amyloid polypeptide (hIAPP$_{1-37}$) and $A\beta_{40}$ by applying the all-atom molecular dynamics (MD) simulations. The random seed simulations revealed the higher toxicity of the δ monomeric isomer and the δε and δδ dimers compared with ε and εε conformations considering the critical role of α-helix in membrane disruption and further transition to the β-sheet structure (Tau and Pi tautomeric forms of histidine are denoted as ε and δ, respectively). In addition, the $A\beta_{40}$(δδδ) isomeric form in cross-seeding with Islet(ε) and Islet(δ) monomers could maintain or enhance the β-sheet formation in its structure that may lead to further aggregation and higher pathogenicity. The other isomer complexes without a β-sheet amount in their monomeric structure, except one seed of the Islet(ε) and $A\beta_{40}$(εεε) complex, did not show the sheet generation within the simulation period. It may display the importance of $A\beta_{40}$(δδδ) isomeric form during disease development. Our computational approach at the atomic level is a different insight into the extrinsic parameter that may affect the T2D and AD formation and the pathological link between them.

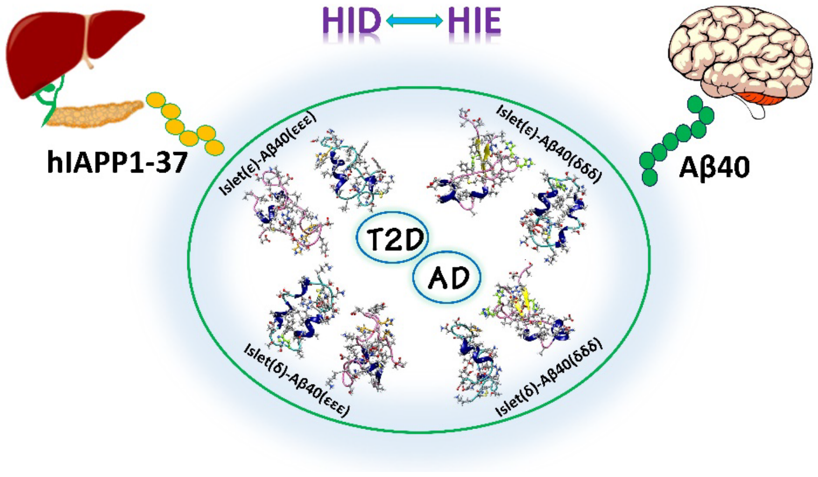

**Figure.** Conformations of $A\beta_{1-40}$/hIAPP$_{1-37}$ isomeric tautomers

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# Multi-state global fitting of the singlet and triplet potential energy surfaces of $H_3^+$. Quantum dynamics calculations.

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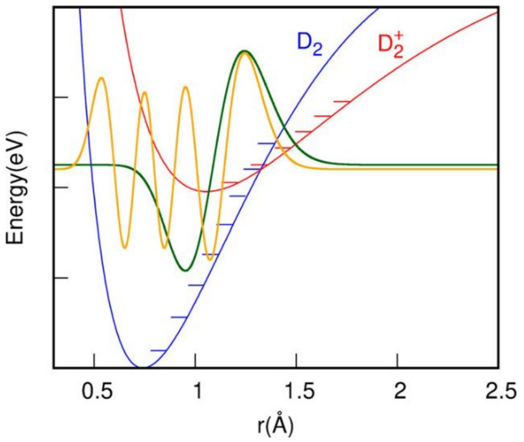
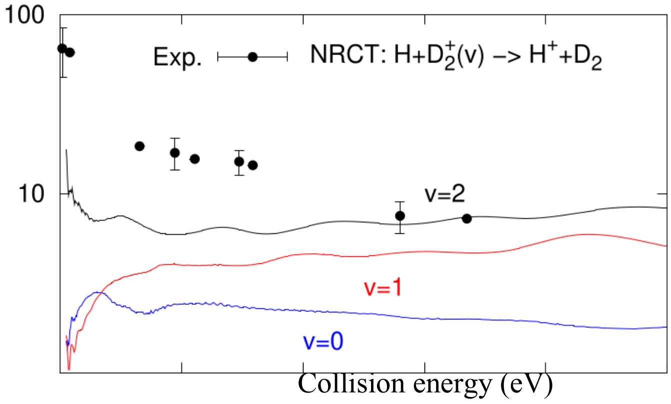
The high interest that $H_3^+$ produces, due to his presence in the interstellar medium[1], is evident from the large number of studies on its spectroscopy and formation, using different techniques. From a theoretical point of view, the Quantum Chemistry of this system is rather simple and very accurate *ab initio* points can be obtained, so that spectra can be reproduced with spectroscopic precision. In the literature there are several global potential energy surfaces for the ground and several excited states of $H_3^+$, although the long range description is still vague. In our group we have applied a new DIM- based multi-state global fitting that provides analytical functions for the diabatic and adiabatic states, and the derivatives and non-adiabatic coupling matrix elements for the three singlet and triplet states. The multi-states global fitting considers the right symmetry for the individual terms of the DIM matrix as well as for the full system, ABB and AAA symmetry respectively. Special attention was taken in the description of the long range interaction, particularly important in the singlet states, where the swapping of the positive charge produces an avoided crossing between the two lowest states in the entrance channel ($H_2 + H^+$).

In this work are presented the details of the fitting method and the accuracy provided by the fit for the three singlet and three triplet states of $H_3^+$. In addition, we present the quantum dynamics calculations for the charge transfer process in the collision reaction $H_2 + H^+$ and its isotopic variants, including the effect of the initial vibrational state of the diatomic molecule.





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# BLACKBODY INFRARED RADIATIVE DISSOCIATION STUDIES OF HYDRATED MAGNESIUM SULFATE CATIONS: $[Mg_n(SO_4)_{n-1}(H_2O)_m]^{2+}$

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Climate change is the most pressing problem nowadays and is likely to remain it in the future. Magnesium sulfate might play a role in both understanding the mechanisms behind climate change and tackling it by the introduction of new technologies. To be specific, $MgSO_4$ could play an important role in the production of sea salt aerosols, as both $Mg^{2+}$ and $SO_4^{2-}$ are common constituents of sea salt aerosols [1]. These again act as cloud condensation nuclei and therefore influence precipitation and the albedo. In the role of mitigating climate change, $MgSO_4$ in the form of epsomite is a promising candidate for being used in energy storage systems. Namely, the hydration and dehydration of $MgSO_4$ can be used to thermo-chemically store solar energy produced in the summer until the winter [2].

In this contribution, dissociation processes in $[Mg_n(SO_4)_{n-1}(H_2O)_m]^{2+}$ are investigated. On the experimental side, blackbody infrared radiative dissociation (BIRD) studies are performed within Fourier Transform Ion Cyclotron Resonance (FT-ICR) mass spectrometry experiment. These experiments show both expected behavior and phenomena that cannot be explained so far. In the collision cell, $Mg_{n+1}(SO_4)_n$ particles are never produced alone. Instead, several water molecules are always attached to it. In the BIRD experiments themselves, the most prominent dissociation pathway is water loss. However, especially for larger $n$, $SO_3$ loss is also observed. Unintuitively, for $[Mg_7(SO_4)_6(H_2O)_6]^{2+}$, $SO_3$ loss is only observed as soon as all six water molecules have been lost. Conversely, for $[Mg_4(SO_4)_3(H_2O)_5]^{2+}$, $SO_3$ loss is already observed as soon as three water molecules are lost. This might be due to inherent structural differences between the two compounds. Besides, for all investigated values of $m$ and $n$, the parent ion does not disappear even after being exposed to blackbody radiation for 30 seconds. This suggests that there are at least two classes of isomers present, respectively, and not all of them dissociate.

By performing quantum chemical calculations, we rationalize these findings and shed light onto the aspects that are not understood well so far. In particular, we analyze the structure of the ions using both standard optimization approaches and genetic algorithm search to find structures that are hard to find solely by chemical intuition, employing semi-empirical and density functional theory (DFT) approaches to describe the potential energy surface. With the minima in hand, we apply multi-well master equation modeling combined with RRKM theory to calculate rate constants of the pathways and to estimate the importance of the isomer distribution on the total dissociation rate constant.

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# Interaction of low energy electrons with isolated and microhydrated favipiravir

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We aim to study the reductive properties of favipiravir as a hopeful candidate for a radiosensitizing agent. Radiosensitizing agents increase the radiotherapy effect. The increase has many sources and one of them can be the reaction of electron attachment (EA). It was shown that biological reactions with reducing character can be related to EA [1]. It was also proven that the electron-reduction characteristics of drugs can influence their transport and binding properties [2]. We study the behaviour of favipiravir in reactions with low-energy electrons (LEE) [3] using electron attachment spectroscopy. We investigate them in their isolated and microhydrated forms. Experimental data are supported by *ab initio* calculations of reaction thresholds. We show that EA to favipiravir undergo mainly the formation of the long-living parent anion and only small fraction leads to dissociative EA. High stability of the generated parent anions is convenient for transport and radiosensitizing purpose. The pattern of the secondary fragmentation pathways was analyzed by threshold DFT and interpreted mainly by reactions on the $CONH_2$ group. EA on hydrated favipiravir $Fav.(H_2O)_n$ leads to dissipation of available energy into the solvent. Our findings affirm that favipiravir could be investigated as a candidate for a radiosensitizers [4].

**Acknowledgments:** This work was supported by Czech Ministry of Education, Youth and Sports, program INTER-EXCELENCE grant number MSMT-21080/2020-34.

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# Determination of the magnetic shielding in light atoms and small molecules

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Theoretical studies of the magnetic shielding are crucial for NMR spectroscopy as it cannot be determined directly from the experiment. According to IUPAC, the magnetic shielding constant of 3-He is the universal reference standard in NMR spectroscopy. This approach unifies multinuclear methods into one NMR spectroscopy because the values of magnetic shielding have the same meaning for all observed nuclei.

In case of light atoms and small molecules, nonrelativistic quantum electrodynamics (NRQED) formalism allows for systematic description of the shielding constant as the sum of the leading and further contributions (e.g. relativistic, QED, nuclear mass corrections). The increasing accuracy in NMR techniques requires consideration of many subtle effects and makes the examination to go beyond the leading contribution.

We will present the latest advances in the determination of the magnetic shielding constant for helium-3 [1] and hydrogen molecules isotopologues [2].

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# Efficient machine learning for excited states properties and property-based diabatization

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The efficiency of machine learning algorithms for electronically excited states is far behind ground-state applications.[1] The reason is mainly the high complexity of reference quantum-chemical calculations, high densities of states and the fact that the modelled properties are not smooth in the vicinity of conical intersections. We propose several statistical data-based techniques to improve the performance of excited-state modelling in the space of nuclear configurations, overcoming the outlined limitations.

The direct application of regression algorithms to each adiabatic state is straightforward but it is usually not very efficient as smooth surfaces are a prerequisite for efficient machine learning. The best performance can be achieved for diabatic states. However, diabatization is an outstanding problem itself. Depending on the symmetry of the intersecting electronic states, we can distinguish several types of intersections with different dimensionalities of the seam space. The states can be simply reordered in the case of symmetry-allowed conical intersections between states of different symmetry. While this is a primitive task in one dimension, it is a complex problem for a multidimensional system, which we tackle by maximizing the regression performance. For more common same-symmetry intersections, we combine our approach with property-based diabatization. Property-based diabatization schemes are usually simple and computationally cheap to apply. However, they typically suffer from several problems: the order of obtained diabatic states is not consistent throughout the nuclear configuration space and the diabatic couplings change signs randomly. We tackle both these problems by extending our machine learning approach to optimize the order and signs of diabatic states and couplings, respectively.

Another option how to increase the efficiency of excited-state simulations in the configuration space is to reduce the number of geometries representing the nuclear density. However, this usually results in a loss of accuracy. We use here a fast quantum chemical method as an exploratory method in combination with simulated annealing to select a subset of geometries that sufficiently represents the whole nuclear distribution for a given problem.[2] By using this approach, we can substantially reduce the accuracy loss and therefore speed up the simulations by an order of magnitude which efficiently allows us to employ better electronic structure methods. While different problems can be tackled using the proposed approach, we show here the performance for electronic spectra simulations based on the nuclear ensemble method.

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# Four-Dimensional Scaling of Dipole Polarizability in Quantum Systems

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Polarizability is a key response property of physical and chemical systems, which has an impact on intermolecular interactions and spectroscopic observables. The calculation of polarizability for quantum systems involves an infinite sum over all excited (bound and continuum) states, concealing the physical interpretation of polarization mechanisms and complicating the derivation of efficient response models. Approximate expressions for the dipole polarizability, α, rely on different scaling laws connecting α to the system-size. We have shown that the general quantum-mechanical system-size dependence of polarizability follows a four-dimensional scaling law instead of the commonly accepted textbook result (classical 3D scaling: $\alpha \sim$ Volume $\sim R^3$, where $R$ is the radius of the system). This unusual four-dimensional scaling is a pure quantum effect stemming from quantum fluctuations, and it is valid for quantum-mechanical systems of varying spatial dimension, symmetry, excitation state. Our unified formula is also applicable to many-particle systems, as shown by accurately predicting the dipole polarizability of 36 atoms, 1641 small organic molecules.

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# Semiclassical theory of the kinetics and dynamics of polyatomic molecule formation by radiative association

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Radiative association (RA) is one of many important processes that contribute to molecule production in dust-poor regions of interstellar space. The description of the scattering process in the presence of a radiation field is challenging. Owing to the elaborate quantum mechanical treatment, most of the previous dynamical calculations have focused either merely on diatomic molecule formation or on a few triatomic systems. Since the quantum dynamics methods are not feasible for larger polyatomic molecules, we have developed two trajectory-based methods in order to characterize the dynamics and kinetics of polyatomic molecule formation through radiative association. One is for RA in absence of electronic transitions based on the classical Larmor theory of radiation, and another for the calculation of RA through electronic transitions based on the semiclassical surface-hopping formalism. Both methods can provide a practical but still efficient solution to obtain quantum state resolved RA cross sections or rate constants for arbitrary polyatomic systems. Furthermore, our methods are not only applicable for the description of RA but it can be used for the semiclassical characterization of any molecular process where either spontaneous or stimulated emission occurs.

# Pickup of hydrogen bonding molecules on benzene clusters

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Benzene (Bz) clusters and their abilities to pickup abundant interstellar molecules are investigated in relevance to astrochemistry on interstellar nanoparticles. [1,2] In our experiment, individual molecules are doped on Bz clusters as they fly in a molecular beam through a pick-up cell. Approximately 3 ms after doping, the clusters are ionized (70 eV) and probed by time-of-flight mass spectrometry. The neutral Bz clusters with embedded molecules are also investigated in the prospect of intracluster reactions triggered by the electron ionization or low-energy (below 10 eV) electron attachment.

In the present experiment, we compared Bz cluster ability to uptake selected hydrogen bonding molecular species from interstellar space medium (ISM), i.e., water $H_2O$, methanol $CH_3OH$ and ethanol $CH_3CH_2OH$. The supersonically expanded mixture of Bz/Argon generated large $(Bz)_N$ clusters ($N \approx 300$) with radius around 2.2 nm, which serves as a model system of PAH clusters to study ISM heterogenous chemistry and ice mantle growth. All the tested molecules exhibit high mobility resulting in cluster formation within 3 ms. This also indicates liquid-like state of the Bz cluster surface. Furthermore, we estimated the relative pickup probability for each hydrogen bonding molecule. Water molecules show around 30% lower probability for pickup compared to methanol and ethanol, which might be of high interest for atmospheric and astrochemical simulations of the nanoparticle growth.[2]

Pick-up and heterogenous chemistry of other interstellar relevant molecules with PAHs clusters and PAHs/water ices will be presented as well.

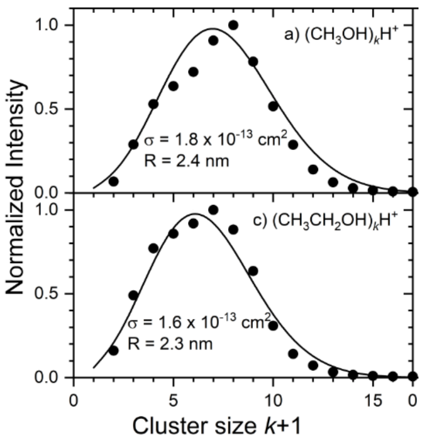

Figure 1: Cluster ion fragment abundances fitted with Poisson distributions.

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# Methane ultra-precise saturation spectroscopy at 1.65 mm with coherence transfer stabilized diode laser CRDS spectrometer

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We present an extensive ultra-high-accuracy study of $CH_4$ overtone transitions in the near IR spectral range near 1.65 um, exploiting sub-Doppler saturation spectroscopy with Comb Coherence Transfer (CCT) stabilized laser source. CCT uses a feed-forward frequency correction to transfer the optical phase of a frequency comb to the beam of a free-running diode laser. This allows effective amplification of selected comb tooth intensity by 50 dB while adding agile and accurate frequency tuning. In the present work, SI-traceable frequency calibration and comb tooth narrowing down to 20 kHz is additionally provided by comb frequency locking to an ultra-stable optical frequency reference distributed from Paris to Grenoble through the RENATER optical fiber network [1]. We apply this CCT broadly tunable source for saturated cavity ring-down spectroscopy of ro-vibrational R0 to R10 multiplets in the 2ν3 band of $^{12}CH_4$ (from 6015 cm$^{-1}$ to 6115 cm$^{-1}$). Due to efficient cavity injection by the spectrally narrow source, large intra-cavity power build-up has been achieved and Doppler-free Lamb dips were observed with high signal/noise as a result of efficient saturation of the ro-vibrational transitions. kHz-accurate transition frequencies are derived improving by three orders of magnitude previous values from spectra in the Doppler regime, which are strongly affected by line blending. While previous saturation spectroscopy investigations addressed specific 2ν3 multiplets (R6 or R9), the CCT approach allowed for a rapid coverage of the entire R0–R10 series. Measured transition frequencies are compared with experimental and theoretical line lists available in the literature [2].

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# Construction of a multi-reflectron for multiply charged helium droplets

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Multiply charged helium nanodroplets (HNDs) show superior characteristics for producing nanoparticles with a narrow size distribution [1]. Both multiply charged HNDs and nanoparticles can be difficult to access with conventional mass spectrometers due to the large mass-to-charge ratios involved. Here, we present a multi-reflectron time-of-flight device (MR-ToF) [2] and its potential applications in ion trapping and mass spectrometry experiments utilizing pristine and doped multiply charged HNDs. The main focus of our recent work is the simulation of ion paths using Simion in order to optimize the experimental setup. Furthermore, experimental results of a possible experiment with this MR-ToF setup are shown [3].

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# Calculation of rotational circular dichroism for diamagnetic and paramagnetic molecules

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Circular dichroism (CD) techniques are invaluable for conformational and enantiomeric analyses of optically active molecules. While CD spectra are routinely measured for electronic and vibrational transitions (ECD and VCD), rotational transitions (RCD) give much weaker signal and they have not been detected so far. To guide future experiments, it may be convenient to identify molecules with high spectral intensities. Salzman [1-4] performed RCD calculations for six small diamagnetic molecules (d1, d2, d3-oxiranes, methyloxirane, methylthiirane, transdimethyloxirane), using the rigid rotor Hamiltonian. Here, we extend on his theory and also calculate RCD spectra for a more biologically relevant molecule, the L-alanyl-L-alanine dipeptide. We show that the quadrupole contribution is zero, while paramagnetic molecules give enhanced RCD signal. Dipole and rotational strengths of the six diamagnetic molecules are investigated up to high rotational quantum numbers ($J \sim 120$), and trends in spectral intensities in dependence on transition frequency and $J$ are analyzed. In general, dipole strength remains constant with growing $J$, while rotational strength rises.

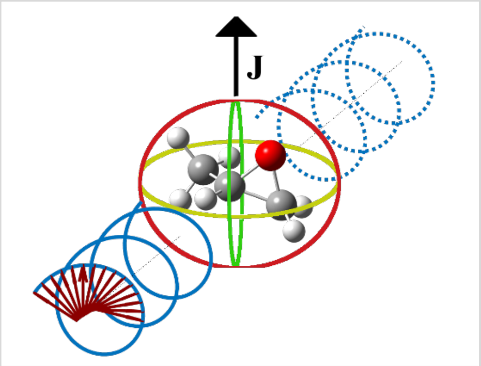

*Figure 2* – Methyloxirane absorbing an incident circularly polarized photon, making it shift its angular momentum ***J***

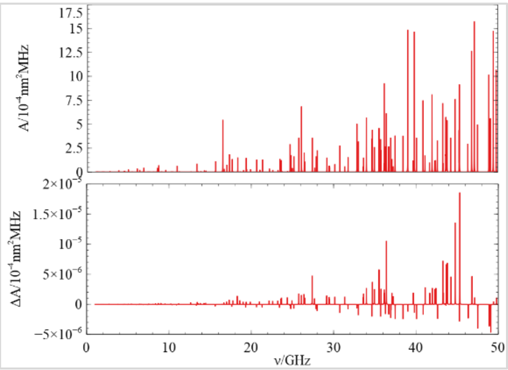

*Figure 3* – Normal absorption and RCD spectrum of methylthiirane

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# Coincidence velocity map imaging using TPX3CAM, a time stamping optical camera with 1.5 ns timing resolution

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We demonstrate a coincidence velocity map imaging apparatus equipped with a novel time-stamping fast optical camera [1], TPX3CAM [2]. Its high sensitivity and nanosecond timing resolution allow for simultaneous position and time-of-flight detection of electrons and ions. This single detector design is simple, flexible, and capable of highly differential measurements. We show detailed characterization of the camera and its application in strong field ionization experiments [3].

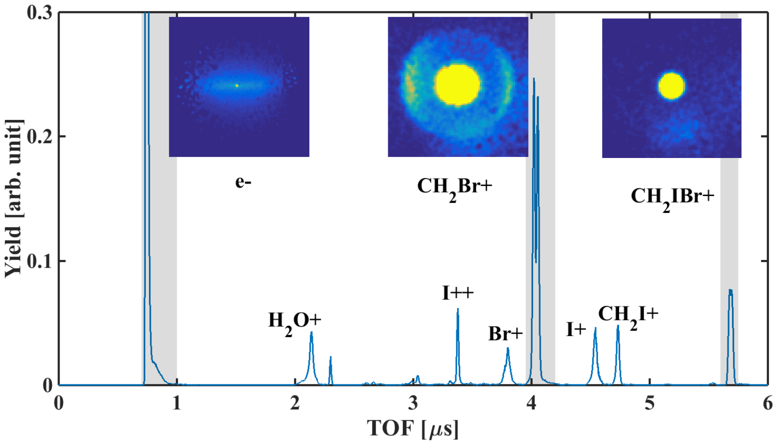

Figure 1. TOF mass spectrum for $CH_2IBr$ following strong field ionization. Momentum distribution are shown for selected fragments.

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