ECAMP14

14th European Conference on Atoms Molecules and Photons

June 27-July 1, 2022

ABSTRACT BOOK

VILNIUS, LITHUANIA

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Content

Conference program

(INV) - invited talk (25 + 5 minutes)
(HT) - hot topics talk (12 + 3 minutes)

Sunday, June 26

Hall: Alfa

15:00-19:00	Registration “Radisson Blu hotel Lietuva” conference center	
16:30-18:30	Walking city tour (meeting point “Radisson Blu hotel Lietuva” lobby	

Monday, June 27

Hall: Alfa

8:00-9:00	Registration and welcome coffee	
9:00-9:15	Welcome greetings (Hall Alfa)	
Plenary Lecture 1 Chair: **Joachim Burgdörfer** **Hall: Alfa**		
9:15-10:00	Light driven ionization processes ... and the role of the photon‘s momentum	Reinhard Dörner Germany (Plen-1)
10:00-10:30	**Coffee break**	
Parallel session (A1) Chair: **Reinhard Dörner** **Hall: Alfa**		
Invited speakers:		
10:30-11:00	First instants following XUV photoionization: attosecond and femtosecond dynamics in molecules, from carbon structures to proteins	Franck Lépine, France (A1-1-INV)
11:00-11:30	Ultrafast spectroscopy of bio-chromophores with few-femtosecond UV pulses	Rocío Borrego Varillas, Italy (A1-2-INV)
11:30-12:00	All-XUV-Optical Nonlinear Absorption Spectroscopy with Free-Electron Lasers	Christian Ott, Germany (A1-3-INV)
12:00-12:30	Attosecond science at the Linac Coherent Light Source: recent developments and future directions	Agostino Marinelli, USA (A1-4-INV)
Parallel session (B1) Chair: **Károly Tőkési** **Hall: Beta**		
Invited speakers:		
10:30-11:00	Highly charged ions interacting with 2D materials	Marika Schleberger, Germany (B1-1-INV)
11:00-11:30	Interaction of trapped atoms with twisted light	Andrey Surzhykov Germany (B1-2-INV)

11:30-12:00	Probing charge-transfer neutralization reactions of atmospheric importance using the ion storage facility DESIREE	Richard Thomas, Sweden (B1-3-INV)
12:00-12:30	Experimental Studies of Nonperturbative Dynamics in Heavy-Ion-Atom Collisions	Pierre-Michel Hillenbrand, Germany (B1-4-INV)
12:30-14:15	**Lunch break**	
Plenary Lecture 2 Chair: **Rosario González-Férez** **Hall: Alfa**		
14:15-15:00	Quantum gases of ultracold polar molecules	Silke Ospelkaus-Schwarzer, Germany (Plen-2)
15:00-15:30	**Coffee break**	
Parallel session (A2) Chair: **Silke Ospelkaus-Schwarzer** **Hall: Alfa**		
Invited speakers:		
15:30-16:00	Ultracold RbCs Molecules: Robust Storage Qubits and Rotationally Magic Traps	Simon L. Cornish, UK (A2-1-INV)
16:00-16:30	Self-Pinning Transition of a Tonks-Girardeau Gas in a Bose-Einstein Condensate	Thomas Busch Japan (A2-2-INV)
16:30-17:00	TBA	Cristiane Morais-Smith, The Netherlands (A2-3-INV)
Hot topics:		
17:00-17:15	A Weakly-Interacting Many-Body System of Rydberg Polaritons based on Electromagnetically Induced Transparency	Ite A. Yu, Taiwan (A2-1-HT)
17:15-17:30	Response of Small Helium Clusters to Strong Laser Fields	Maksim Kunitski, Germany (A2-2-HT)
Parallel session (B2) Chair: **Darius Abramavičius** **Hall: Beta**		
Invited speakers:		
15:30-16:00	Absolute Measurement of a THz Transition Frequency Referenced to a Magnetic Dipolar Transition in Ca+ ion	Caroline Champenois, France (B2-1-INV)
16:00-16:30	Extending coherent multidimensional spectroscopy to new target systems and new light sources	Lukas Bruder, Germany (B2-2-INV)
16:30-17:00	Terahertz Frequency	Luigi Consolino, Italy (B2-3-INV)
Hot topics:		
17:00-17:15	Quantitative Study of Enantiomer-Specific State Transfer	Johannes Bischoff, German (B2-1-HT)
17:15-17:30	K-LL Auger Decay of Doubly Excited States of Argon	Matjaz Žitnik, Slovenia (B2-2-HT)
17:30-19:15	**Poster session 1 and coffee break**	
19:15-21:30	Welcome Party	

Tuesday, June 28

Hall: Alfa

8:00-9:00	Registration and welcome coffee	
Plenary Lecture 3 Chair: **Gediminas Juzeliūnas** **Hall: Alfa**		
9:00-9:45	Attoscience and Quantum Information	Maciej Lewenstein, Spain (Plen-3)
9:45-10:15	**Coffee break**	
Parallel session (A3) Chair: **Wen-Te Liao** **Hall: Alfa**		
Invited speakers:		
10:15-10:45	Molecular polaritonics and subwavelength cavity QED	Johannes Feist, Spain (A3-1-INV)
10:45-11:15	New Perspectives on Quantum Geometry, Super-conductivity and Bose-Einstein Condensation	Päivi Törmä, Finland (A3-2-INV)
11:15-11:45	Quantum light-induced nonadiabaticity in molecular systems	Agnes Vibok, Hungary (A3-3-INV)
11:45-12:15	A fresh perspective on the Casimir effect	Almut Beige, United Kingdom (A3-4-INV)
Parallel session (B3) Chair: **Marika Schleberger** **Hall: Beta**		
Invited speakers:		
10:15-10:45	Spectroscopy of helium-tagged molecular ions	Elisabeth Gruber, Austria (B3-1-INV)
10:45-11:15	Environmental Effects on Electron Attachment	Jaroslav Kočišek, Czech Republic (B3-2-INV)
11:15-11:45	Charge migration in betaine by impact of fast atomic ions	Patrick Rousseau, France (B3-3-INV)
11:45-12:15	Ultrafast Processes in Amino-Acids, Amino-Acids Derivatives and Clusters of Amino-Acids Induced by Ionizing Radiation	Sergio Diaz-Tendero, Spain (B3-4-INV)
12:15-14:00	**Lunch break**	
Plenary Lecture 4 Chair: **Daniela Rupp** **Hall: Alfa**		
14:00-14:45	Probing Nuclear Dynamics with Electron Scattering	Juraj Fedor, Czech Republic (Plen-4)
14:45-15:15	**Coffee break**	
Parallel session (A4) Chair: **Agnes Vibok** **Hall: Alfa**		
Invited speakers:		

15:15-15:45	High Resolution Resonant Auger Spectroscopy of Ultrafast-decaying. Core-ionized Atoms	Tommaso Mazza, Germany (A4-1-INV)
15:45-16:15	Attosecond Science at the FERMI Free Electron Laser	Carlo Callegari, Italy (A4-2-INV)
16:15-16:45	Two-Color X-Ray Pump-Probe Spectroscopy at SwissFEL	Kirsten Andrea Schnorr, Switzerland (A4-3-INV)
Hot topics:		
16:45-17:00	Anisotropic dynamics of two-photon ionization: real time imaging of photoemission	Jérémie Caillat, France (A4-1-HT)
17:00-17:15	Rabi Dynamics Driven by a Seeded FEL at XUV-wavelengths	Mattias Bertolino, Sweden (A4-2-HT)
Parallel session (B4) Chair: **Krzysztof Sacha** **Hall: Beta**		
Hot topics:		
15:15-15:30	Wave-packet dynamic in a SU(2) non-Abelian Gauge field	Wilkowski David, Singapore (B4-1-HT)
15:30-15:45	Quantum fluids of light in hot atomic vapors	Tangui Aladjidi, France (B4-2-HT)
15:45-16:00	Manifestation of relative phases in collision of BoseBose droplets	Mariusz Gajda, Poland (B4-3-HT)
16:00-16:15	Precision Measurements and Pauli Blocking with Quantum Degenerate Metastable 3He	Yuri van der Werf, The Netherlands (B4-4-HT)
Invited speakers		
16:15-16:45	Non-equilibrium state preparation in driven-dissipative atomic quantum gases	André Eckardt, Germany (B4-1-INV)
16:45-17:15	Synthetic Gauge Fields with Ultracold Atoms	Monika Aidelsburger, Germany (B4-2-INV)
17:10-19:00	**Poster session 2 and coffee break**	
Public lecture Chair: **Gediminas Juzeliūnas** **Hall: Alfa**		
19:15	Time, Einstein and the coolest stuff in the universe	William Phillips, USA (Pub-Lect-1)

Wednesday, June 29

8:00-9:00	Registration and welcome coffee	
Plenary Lecture 5 Chair: **Francesco Saverio Cataliotti Cataliotti** **Hall: Alfa**		
9:00-9:45	Dynamically symmetry breaking in a bipartate optical lattice	Ian B. Spielman, USA (Plen-5)
9:45-10:35	CONFERENCE PHOTO **Coffee break**	
Young Scientist Prize Lecture Chairs: **Maciej Lewenstein, Joachim Burgdörfer** **Hall: Alfa**		
10:35-11:30	Young Scientist Prize Award Ceremony and Lecture by Jordi Tura i Brugués " Detecting Bell correlations in quantum many-body systems"	Jordi Tura i Brugués, The Netherlands (Plen-6)
11:30–12:05	AMOPD General Assembly	
12:05–12:45	EGAS General Assembly	
12:45-14:00	**Lunch**	
14:00	Option 1: Tour to Trakai Castle; Option 2: Visit to Laser company "Light conversion" and Labs of Dept. Phys. of Vilnius university; Meeting point: Radisson Blu hotel lobby (1st floor)	
19:30	**Conference dinner** 19:15 Busses will leave Radisson BLU hotel, meeting point hotel lobby (1st floor)	

Thursday, June 30

8:00-9:00	Registration and welcome coffee	
Plenary Lecture 7 Chair: **Hélène Perrin** **Hall: Alfa**		
9:00-9:45	Spatiotemporal Control of Brain Function Using Holographic	Valentina Emiliani, France (Plen-7)
9:45-10:15	**Coffee break**	
Parallel session (A5) Chair: **Christophe Blondel** **Hall: Alfa**		
Invited Speakers:		
10:15-10:45	Probing of the ground-state atomic alignment-to-orientation conversion in an external magnetic field with different polarizations of the probe beam	Marcis Auzinsh, Latvia (A5-1-INV)
10:45-11:15	Dual Comb Spectroscopy for Electronic Fingerprinting	Birgitta Schultze-Bernhardt, Austria (A5-2-INV)
11:15-11:45	Cavity mode-dispersion spectroscopy	Roman Ciurylo, Poland (A5-3-INV)
11:45-12:15	A Decade with Quantum Biology: How Non-Trivial is Quantum Mechanics of Photosynthetic Light-Harvesting?	Tomáš Mančal, Czech Republic (A5-4-INV)
Hot topic:		
12:15-12:30	Reversing time with ultra-cold atoms for quantum undo operations	Ivana Mastroserio, Italy (A5-1-HT)
Parallel session (B5) Chair: **Mikhail Ivanov** **Hall: Beta**		
Invited Speakers:		
10:15-10:45	Towards attosecond imaging at the nanoscale using extreme ultraviolet high harmonic sources	Jan Rothhardt, Germany (B5-1-INV)
10:45-11:15	Influence of Shape Resonances on the Angular Dependence of Molecular Photoionization Delay	Fabian Holzmeier, France (B5-2-INV)
11:15-11:45	Tightly-Focused Elliptically Polarized Light: a Highly Efficient Tool for Chiral Discrimination	Laura Rego, UK (B5-3-INV)
11:45-12:00	Observing the complex dynamics in uracil via simulated XUV spectra	Lena Bäuml, Germany (B5-4-INV)
Hot topic:		
12:00-12:15	Sub-cycle Optical Pulses Generated via Parallel Parametric Waveform Synthesis for Attosecond Science	Roland E. Mainz, Germany (B5-1-HT)
12:30-14:00	**Lunch break**	
Plenary Lecture 8 Chair: **Franck Lépine** **Hall: Alfa**		
14:00-14:45	Atomic Physics at FAIR: Quantum Dynamics in Extreme Electromagnetic Fields	Thomas Stöhlker, Germany (Plen-8)

14:45-15:15	**Coffee break**	
Parallel session (A6) Chair: **Thomas Stöhlker** **Hall: Alfa**		
Invited Speakers:		
15:15-15:45	Studies of reactive and inelastic collisions in a cryogenic multipole trap	Robert Wild, Austria (A6-1-INV)
15:45-16:15	New Insights on The Ozone Formation	Marjan Mirahmadi, Germany (A6-2-INV)
16:15-16:45	X-rays from the Universe	Jörn Wilms, Germany (A6-3-INV)
Hot topics:		
16:45-17:00	A Levitating Droplet as a Toy Atom	Javier Tello Marmolej Sweden (A6-1-HT)
17:00-17:15	Experimental study of X-ray photon-induced desorption from molecular ices: indirect mechanism and astrophysical implications	Romain Basalgète, France (A6-2-HT)
Parallel session (B6) Chair: **Karolina Słowik** **Hall: Beta**		
Invited Speaker:		
15:15-15:45	Nonlinear optical phenomena from high repetition rate lasermatter interactions in transparent solids	Audrius Dubietis, Lithuania (B6-1-INV)
Hot topics:		
15:45-16:00	High-resolution manipulation and imaging of cold atoms through a multimode fiber	Sébastien Garcia, France (B6-1-HT)
16:00-16:15	Partial cross sections for mutual neutralization involving H− and D−	Arnaud Dochain, Belgium (B6-2-HT)
Invited Speaker:		
16:15-16:45	The Fate of Knockout- Damaged PAHs and Fullerenes: Bridging Ultrashort and Ultralong Timescales	Michael Gatchell, Sweden (B6-2-INV)
Hot topics:		
16:45-17:00	Progress towards a molecular lattice clock to search for time-variation of the proton-to-electron mass ratio	Jonas Rodewald, UK (B6-3-HT)
17:00-17:15	The origin of enhanced O2 + production from photoionized CO2 clusters	Smita Ganguly, Sweden (B6-4-HT)
17:15-19:00	**Poster session 3 and coffee break**	

Friday, July 1

Hall: Alfa

8:00-9:00	Registration and welcome coffee	
Plenary Lecture 9 Chair: **Alicia Palacios** **Hall: Alfa**		
9:00-9:45	Lightwave Electronics in Trivial, Topological, and Strongly Correlated Solids	Mikhail Ivanov, Germany (Plen-9)
9:45-10:15	**Coffee break**	
Parallel session (A7) Chair: **Almut Beige** **Hall: Alfa**		
Invited speakers:		
10:15-10:45	Realizing a topological gauge theory in an optically dressed Bose-Einstein condensate	Leticia Tarruell, Spain (A7-1-INV)
10:45-11:15	Speeding up a trapped ion quantum processor via Rydberg interaction	Markus Hennrich, Sweden (A7-2-INV)
11:15-11:45	Mott-squeezed states with ultra-cold fermions	Emilia Witkowska, Poland (A7-3-INV)
11:45-12:15	Rydberg molecules : spectra and scattering properties	Shuhei Yoshida, Austria (A7-4-INV)
Parallel session (B7) Chair: **Hélène Perrin** **Hall: Beta**		
Invited speakers:		
10:15-10:45	Accurate determination of the fine-structure constant using atom interferometry	Saida Guellati-Khélifa, France (B7-1-INV)
10:45-11:15	Ultrastable frequency transfer through optical fiber links at the continental scale	Anne Amy-Klein, France (B7-2-INV)
11:15-11:45	Towards stimulated decay of antihydrogen atoms	Chloé Malbrunot, Switzerland (B7-3-INV)
11:45-12:15	An Apparatus for the Production of Squeezed Momentum State Superpositions in Atom Interferometers	Leonardo Salvi, Italy (B7-4-INV)
12:15-14:00	**Lunch break**	
Parallel session (A8) Chair: **Mažena Mackoit-Sinkevičienė** **Hall: Alfa**		
14:00-15:30	EPS Young Minds Session	
14:00-14:20	The European Research Council – funding opportunities for bright minds	Christian Oswald, Belgium (A8-1-YMS)
14:20-14:40	Hybrid GaSb/Si spectroscopic sensing technology as a generic technology platform for next-generation IoT and health applications	Augustinas Vizbaras, Lithuania (A8-2-YMS)
14:40-15:00	Career Opportunities in the Scientific and Industrial Laser Technologies	Gediminas Račiukaitis, Lithuania (A8-3-YMS)

15:00-15:20	Discover Modern Trends in Optoelectronics Research at FTMC: Materials, Technology and Applications for Terahertz Photonics	Gintaras Valušis Lithuania (A8-4-YMS)
15:30	Closing	
Parallel session (B8) Chair: **Gediminas Gaigalas** **Hall: Beta**		
Invited speakers:		
14:00-14:30	Recent Developments of NIST Atomic Databases and Online Tools	Yuri Ralchenko, USA (B8-1-INV)
14:30-15:00	Magnetometry with a nanometric-thin K vapor cell	Rodolphe Momier, France (B8-2-INV)
15:00-15:30	Competitive Dehydrogenation and Backbone Fragmentation of Super-Hydrogenated PAHs	Mark Stockett, Sweden (B8-3-INV)
15:30-16:00	**Coffee break**	
Closing ceremony; Concert by Petras Vyšniauskas (saxophone) and Aleksandra Žvirblytė (piano) in Hall Alfa		

PLENARY ABSTRACTS

Light driven ionization processes
… and the role of the photon‘s momentum

Reinhard Dörner

Germany

The talk will discuss recent experiments on the role of the photon momentum in atomic and molecular ionization processes across a huge range of wavelength. The three experiments presented show the breadth of fascinating quantum effects connected with what in a particle picture is the photon momentum and in a wave picture is the spatial dependence of the electromagnetic part of the wave, the magnetic field connected to it and the finite phase velocity of the wave and the nondipole effects resulting from them. The three experiments concern:

1) New insight into Compton scattering with keV photons

2) The discovery of a zeptosecond birth time delay of the photoelectron wave emitted from a molecular orbital in single photon processes

3) The recently observed directional dependence of the energy of the above threshold ionization peaks in the electron energy distribution in multiphoton and strong field ionizations in laser pulses.

References:

1) Kircher et al. Kinematically complete experimental study of Compton scattering at helium atoms near the threshold Nat. Phys., 16 (2020) 756–760

2) Grundmann et al. Zeptosecond Birth Time Delay in Molecular Photoionization Science, 370 (2020) 339-341

3) Lin et al. Photoelectron energy peaks shift against the radiation pressure in strong-field ionization Sci. Adv., vol. 8 no. 12 (2022)

PLEN-2

Quantum gases of ultracold polar molecules

Prof. Dr. Silke Ospelkaus-Schwarzer

Leibniz Universität Hannover Institut für Quantenoptik
Germany

In recent years, tremendous progress in the preparation and control of ultracold molecular gases in the quantum regime has been achieved and has opened exciting new research opportunities. Molecules rotate and oscillate and therefore offer many more quantum degrees of freedom than their atomic counterparts. Polar molecules interact via strong and long-range anisotropic interactions. These unique molecular properties lead to largely unexplored new possibilities and surprising results. These range from peculiar scattering properties via the control of ultracold collisions and chemical reactions to strongly correlated dipolar quantum many-body systems.

Within my talk, I will take you on a tour through recent experiments with ultracold polar molecules.

Attoscience and Quantum Information

M. Lewenstein[1;2]

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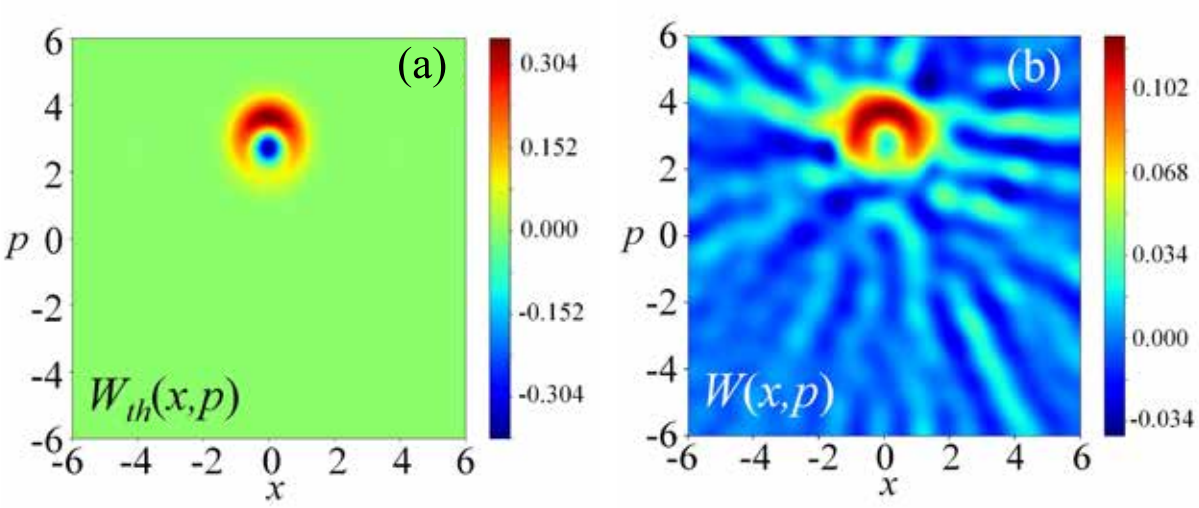

Figure 1: High-photon number optical cat state created by conditioning on HHG. (a) Theoretical prediction for the Wigner function according to [1]. (b) Experimental reconstruction of the Wigner function with mean photon number hni 9:4 0:1, which shows an optical Schrödinger cat state.

In my lecture I will focus on ATTOQUIS, the new joint project of ICFO, FORTH, Technion, CEA, and IOTA toward a symbiosis of attoscience (AS) and quantum information (QI). This is in particular aimed at studying the generation of entangled/quantum correlated states using conditioning methods. I will describe our joint eorts to generate Schrödinger cat states (SCS) of photons conditioned on high harmonic generation (HHG) [1] (see Fig. 1) and/or above threshold ionization. I will also talk about generation of topological order using laser pulses with orbital angular momentum (OAM). I will also discuss HHG as a tool to detect phase transitions and topological in strongly correlated systems. If time permits, I will speculate about measurement of entanglement of OAM of electrons in double ionization, and violation of Bell inequalities by SCS states.

Contemporary Quantum Technologies face major diculties in fault tolerant quantum computing with error correction, and focus instead on various shades of quantum simulation (Noisy Intermediate Scale Quantum, NISQ) devices, analogue and digital Quantum Simulators and quantum annealers. There is a clear need and quest for such systems that, without necessarily simulating quantum dynamics of some physical systems, can generate massive, controllable, robust, entanglement and superpositions states. This will in particular allow the use of decoherence in a controlled manner, enabling the use of these states for quantum communications (e.g. to achieve ecient transfer of information in a safer and quicker way),

quantum metrology, sensing and diagnostics (e.g. to precisely measure phase shifts of light elds, or to diagnose quantum materials). In the ATTOQUIS project, we propose an answer to these needs, by opening new avenues for QI science in symbiosis with Attoscience (AS) and Quantum Optics (QO). To date, there are no existing platforms that can bring processes at such short time-scales to Quantum Information systems. ATTOQUIS aims at realizing a set of stable and reproducible methods to generate massive entangled states and massive quantum superpositions. This will be accomplished by: i) Studying the generation of entangled/ quantum correlated states using conditioning methods; ii) Studying strong-eld physics and atto-second science driven by quantum light; iii) Studying quantitative and measurable eects of decoherence in atto-science.

References

[1] M. Lewenstein, M.F. Ciappina, E. Pisanty, et al., \Generation of optical Schrödinger cat states in intense laser{matter interactions", Nature Phys. 17, 1104{1108 (2021).

Probing Nuclear Dynamics with Electron Scattering

Juraj Fedor

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One of the central tasks in AMO physics is to specify how the atomic nuclei move, for example, upon a vertical excitation by an external trigger. In this talk I will focus on the excitation mediated by collisions of molecules with free electrons. The interaction time of an electron with the kinetic energy in the chemical range (units of eV) is, in the direct scattering regime, typically too short for any nuclear dynamics. The situation changes if quasi-bound states embedded in the continuum are formed in the collision. Such states – electronic resonances and virtual states – have often autodetachment lifetime comparable with the timescale of nuclear motion. Probing various decay channels of the continuum states thus provides information about the nuclear dynamics.

The main experimental tools are a two-dimensional electron energy loss spectroscopy and a velocity-map-imaging dissociative electron attachment spectroscopy. The first technique provides information about the initial states of nuclear motion via measuring the energies of detached electrons, prior to molecular dissociation. The second technique provides information about the kinematics and dynamics of anionic fragments and thus about the final stage of the nuclear motion. I will provide an overview of effects which are revealed by the combination of these two techniques. The examples include an extremely non-Born-Oppenheimer dynamics of the vibronic coupling through continuum, vibrational autodetachment mediated by a presence of dipole-bound states, or structure-dynamics relationship of core-excited resonances.

PLEN-5

Dynamically symmetry breaking in a bipartate optical lattice

Ian B. Spielman

Fellow, Joint Quantum Institute
National Institute of Standards and Technology and the University of Maryland

Topological invariants robustly classify gapped quantum systems in equilibrium, and phenomena such as the quantized Hall effect---the progenitor of the von Klitzing constant---are macroscopic refections of these invariants.

In addition to dimensionality, the presence or absence of symmetries determines the possible topological invariants. Thus, these invariants remain constant provided that no gaps close and no symmetries are added or removed. For this reason, one might expect the topology of a dynamical quantum system to be similarly robust; this expectation is untrue. Instead as a system undergoes far from equilibrium evolution symmetries come and go, allowing the topology to change as well. We experimentally study these dynamics with ultracold atoms in a 1D bipartite lattice in terms of the Zak phase and a chiral winding number.

Detecting Bell correlations in quantum many-body systems

J. Tura1

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Local measurements on quantum systems may display correlations that escape the paradigm of local realism, as they cannot be explained by any local hidden variable model (LHVM). In other words, such correlations, termed nonlocal, cannot be reproduced by any local deterministic strategies, even if assisted by shared randomness. Bell inequalities bound the space of LHVM correlations and, beside their fundamental interest, these are a resource enabling novel quantum information processing tasks. Bell inequalities define experimentally observable quantities to detect non-locality. In general, they involve correlation functions of all the parties. Unfortunately, these measurements become hard to implement for systems consisting of many constituents, where only few-body correlation functions are typically accessible.

In this talk I am going to review recent progress in the detection of Bell correlations in quantum many-body systems, demonstrating that higher-order correlation functions are not necessary to certify nonlocality in quantum many-body systems. I will construct classes of Bell inequalities capable of revealing Bell correlations out of one- and two-body correlation functions which obey some symmetries, for an arbitrary number of parties [1, 2]. I will review how these inequalities can reveal nonlocality in physically relevant systems, as well as experimental progress in revealing Bell correlations in mesoscopic systems [3, 4]. To conclude, I will review the most recent developments in the field of Bell correlations in quantum many-body systems, such as construction of device-independent witnesses of entanglement depth [5, 6] and data-driven methods for nonlocality detection which allow to find which classes of Bell inequalities are violated given experimental data, thus bypassing the combinatorial optimization problem intrinsic to solving the LHVM polytope in a scalable way [7].

References

[1] Jordi Tura, Remigiusz Augusiak, Ana Belén Sainz, Tamás Vértesi, Maciej Lewenstein and Antonio Acín, Detecting nonlocality in many-body quantum states, Science **344**, 6189, 1256 - 1259 (2014).

[2] Jordi Tura, Gemma de las Cuevas, Remigiusz Augusiak, Maciej Lewenstein, Antonio Acín and Juan Ignacio Cirac, Energy as a detector of nonlocality of many-body spin systems, Phys. Rev. X **7**, 021005 (2017)

[3] Roman Schmied, Jean-Daniel Bancal, Baptiste Allard, Matteo Fadel, Valerio Scarani, Philipp Treutlein, Nicolas Sangouard, Bell correlations in a Bose-Einstein condensate, Science **352,** 6284, 441-444 (2016)

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Spatiotemporal Control of Brain Function Using Holographic Light Shaping and Optogenetics

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The optogenetics revolution began with the discovery of microbial opsins and their sensitivity to light (1971-on), and continued with the demonstration of their utility and function in neuronal cells (2005-on)[1]. Light-induced conformational changes in opsins allow direct transduction of photonic energy into electrical currents, thereby activating or inhibiting neuronal signals in a non-invasive manner. Optogenetics has found use throughout neuroscience because it enables scientists to establish the role of specific cell types in the control of behaviors or pathologies.

Most of these experiments have used relatively simple illumination methods, e.g. using visible light to illuminate large regions of the brain and genetic targeting strategies to 'isolate' a specific cell type. However, this kind of illumination can only synchronously activate entire populations of neurons, thereby controlling them as a whole – a highly unnaturalistic state, given that neurons fire in very complex patterns and sequences as they compute. Indeed, if one examines the activity of a neuronal circuit under physiological conditions, it is characterized in most cases by the fact that even genetically identical cells can have completely independent patterns of activity: each cell in the circuit has its own spatiotemporal signature.

Mimicking and manipulating neuronal activity with this degree of precision has required the development of new optical methods capable of illuminating one or more cells independently in space and time. Today, joint progress in opsin engineering, wave front shaping and laser development have provided the methodology to reach this degree of precision and can control single or multiple target activity independently in space and time with single-neuron and single-spike precision, at large depths. Precisely, a large number of variants in microbial opsins have been recently engineered, to speed-up their kinetics, improve their conductance, confine their expression and shift their absorption peak. In parallel, advanced wavefront shaping approaches combined with two-photon excitation have been developed to precisely guide light through tissues using either scanning or holographic light shaping [2] combined with temporal focusing [3]. Furthermore, the combination of holographic light multiplexing with ad hoc spatiotemporal shaping approaches have been demonstrated to have the capability to generate patterned illumination at multiple axially distinct planes, thus enabling optical control of multiple targets within a 3D volume.

All in all, these progresses have brought optogenetics into a new phase, that we termed few years ago circuit optogenetics [4], offering the possibility for a number of new exciting experimental paradigms e.g., to investigate which is the temporal bounds of functional connectivity within which neurons "fire and wire together", or how many targets need to be activated to perturb complex behavioral responses or yet how large neuronal ensembles, eventually spanning across multiple cortical layers, are functionally connected. Here, we will review the most significant breakthroughs of the past years, which enable circuits manipulation and will show few examples where circuit optogenetics has been used for precise neuronal circuits interrogation.

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Atomic Physics at FAIR: Quantum Dynamics in Extreme Electromagnetic Fields

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Relativistic interactions with matter involving heavy high-Z ions provide a unique testing ground for our understanding of quantum electrodynamics and correlation in the non-perturbative regime as well as of elementary atomic processes mediated by ultrafast electromagnetic interactions. For this realm of physics, the future international accelerator Facility for Antiproton and Ion Research (FAIR) has key features that offer a range of novel challenging research opportunities [1,2]. The facility currently under construction will provide the highest intensities for relativistic beams of both stable and unstable heavy nuclei at high nuclear charge, in combination with the strongest possible electromagnetic fields, thus allowing to extend atomic spectroscopy virtually up to the limits of atomic matter. At the same time, experiments at relativistic beam energies are complemented by experiments at low beam energies (< 10 MeV/u) or even at rest but still at high charge state (see Figure). This scenario is worldwide unique and will deliver high-accuracy data for bound state QED (avoiding Doppler shifts) as well as the determination of fundamental constants. In addition, atomic collisions can be studied in the non-perturbative, adiabatic regime, and even super-critical fields will get accessible

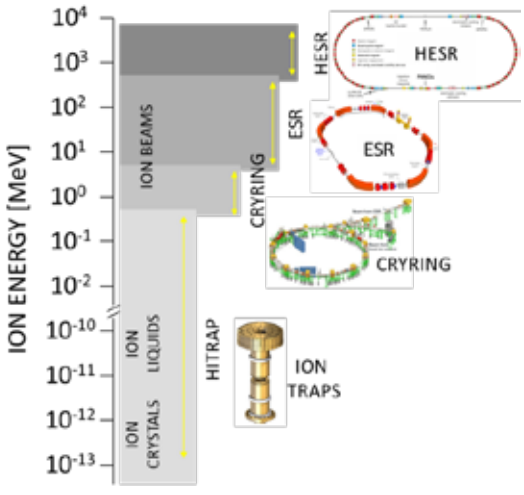

FIG. 1: Figure: Portfolio of storage and trapping facilities at FAIR. Note, HITRAP, CRYRING, and ESR are already in operation or under commissioning.

In this talk, I will also review recent experimental results for atomic, quantum and fundamental research obtained at the already existing ion storage and trapping facilities [3,4]. Examples include e.g. laser spectroscopy exploiting the large Doppler boost associated with relativistic ions as well as precision x-ray, laser and di-electronic recombination spectroscopy. Finally, experiments at the border between atomic and nuclear physics will be addressed in addition with emphasis on rare nuclear decay modes only possible at high atomic charge states.

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Lightwave Electronics in Trivial, Topological, and Strongly Correlated Solids

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Modern light generation technology has evolved to the point where a theorist may reasonably expect an experimentalist to generate light pulses where individual oscillations of the electric field are shaped almost at will. Control of the carrier-envelope phase of few-cycle pulses is now almost routine. One can also reliably generate complex polarization states in two and three dimensions, sculpting the Lissajous figures drawn by the electric field vector during a single optical cycle. As these fields can be made strong enough to compete with the internal electric fields in a medium, coherent electronic motion can be excited and shaped almost at will, at the time-scale of a single light oscillation.

How can we use such opportunities? What happens to a crystal exposed to such light? Do we change its effective band structure and density of states? Can these changes be controlled?

To address these question, I will consider several examples where our ability to control light on the sub-cycle time-scale leads to interesting results.

The first example is PHz valleytronics, which aims to use light to generate coherent electronic excitations in a desired valley of a Brillouin zone. In gapped graphene-type materials, the selection of a desired valley is typically achieved using circularly polarized pulses. I will present our new results [1] which show how a sequence of linearly, not circularly, polarized few-cycle pulses can be used to excite a desired valley in a two-dimensional gapped graphene material such as hexagonal Boron Nitride, then de-excite it, then switch the excitation to another valley, and finally read-out the results in an all-optical manner, all within about 10-20 fs. I will also show that even a single linearly polarized few-cycle pulse can generate selective valley excitation [2], and that PHz valleytronics is possible even in pristine graphene [3], a medium where selective valley excitation was thought to be impossible.

I will then present our new results on lightwave control of electronic excitations and metal-insulator phase transition in a two-dimensional Hubbard system. We find that, in a 2D Hubbard model with strong on-site interaction, a few-cycle laser pulse converts an initially metallic state into a Mott-insulating or a bad metallic state. At high field strength, the density of correlated states is strongly modified by the field. Importantly, this newly “minted” density of states survives after the end of the laser pulse: it appears that the re-shaped charge distribution generates a new self-consistent potential supporting new density of states [4].

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PUBLIC LECTURE ABSTRACT

Time, Einstein and the coolest stuff in the universe

William D. Phillips

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At the beginning of the 20th century Einstein changed the way we think about Time. Now, early in the 21st century, the measurement of Time is being revolutionized by the ability to cool a gas of atoms to temperatures millions of times lower than any naturally occurring temperature in the universe. Atomic clocks, the best timekeepers ever made, are one of the scientific and technological wonders of modern life. Such superaccurate clocks are essential to industry, commerce, and science; they are the heart of Satellite Navigation Systems (satnave), which guide cars, airplanes, and hikers to their destinations. Today, the best primary atomic clocks use ultracold atoms, achieve accuracies of a few seconds in 300 million years, while a new generation of atomic clocks is leading us to re-define what we mean by time. Super-cold atoms, with temperatures that can be below a billionth of a degree above absolute zero, use, and allow tests of, some of Einstein's strangest predictions.

This will be a lively, multimedia presentation, including exciting experimental demonstrations and down-toearth explanations about some of today's hottest (and coolest) science.

FIG. 1: "Time, Einstein and the Coolest Stuff in the Universe" provides a fun and educational overview on how fundamental research influences our daily life.

INVITED, EPS YOUNG MINDS AND HOT TOPIC ABSTRACTS

First instants following XUV photoionization: attosecond and femtosecond dynamics in molecules, from carbon structures to proteins

Franck Lépine

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Ultrashort XUV pulses allow to track the dynamics of electrons and nuclei with extreme precision. In the past few years the development of attosecond experiments gave access to charge dynamics on Angstrom length scale. While these technics have become extremely accurate to describe electron dynamics in atoms and small molecular systems, they remain to be developed for larger molecular structures for which experimental as well as theoretical challenges have to be overtaken. Here we will present recent results from our lab where the electron scattering occurring during the photoionization of carbon based molecules are measured on the attosecond timescale. This shows how attosecond photoelectron interferometry can be used to measure attosecond delays in photoionization and to characterize the hole created upon XUV interaction. The next challenge is to explore the first few femtoseconds following electron loss in large systems. We will show examples of such experiments in the case of proteins. Further developments are ongoing to understand photoionization in complex systems, at the atomic level, offering promises for electron attosecond coherent control in large systems.

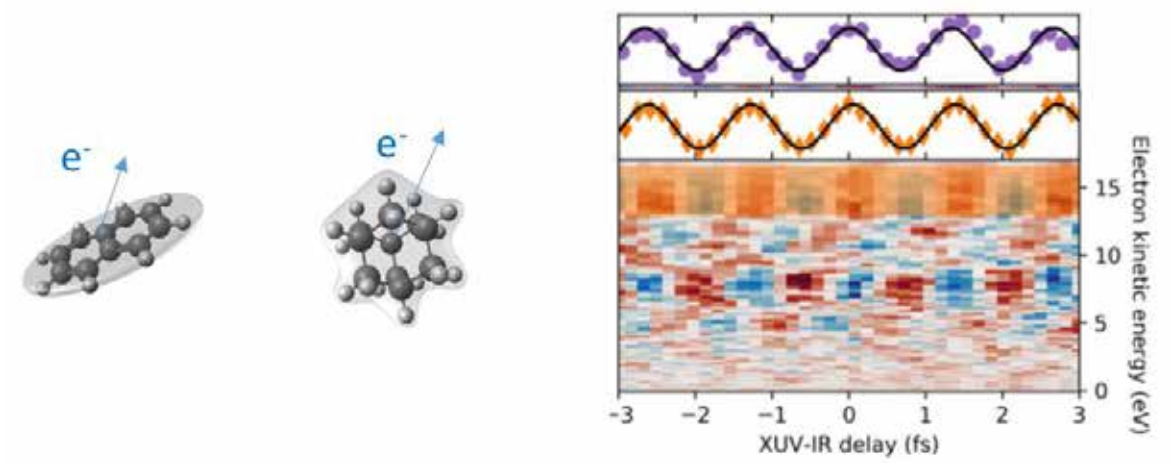

FIG. 1: Comparison between the attosecond delay in photoionization in two molecular structures. Attosecond electron interferometry (RABBITT) is used to measure the electron scattering phase of photoelectrons ejected from the molecules. The phase variation provides a direct information on the hole created in the molecule.

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Ultrafast spectroscopy of bio-chromophores with few-femtosecond UV pulses

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Many molecules of biological interest, such as amino acids or DNA bases, present strong absorption bands in the ultraviolet (UV) spectral range. The primary steps after photo-excitation typically occur in ultrafast time scales - ranging from tens of femtoseconds (fs) down to hundreds of attoseconds - and ultimately determine the system response. The investigation of these processes has been hindered until recently due to technical challenges to access the UV range with enough temporal resolution [1]. In this talk I will present our recent developments on the generation of few-fs UV pulses and their application for ultrafast spectroscopy of DNA bases.

When UV radiation is absorbed by DNA, the electronic energy acquired by the molecule is efficiently converted into vibrational energy on an ultrafast timescale, preventing photochemical reactions which might induce mutations or strand breaks. In those ultrafast processes, conical intersections (CIs) play a crucial role. We have recently tracked the passage of the wavepacket through a CI in uridine (Urd) and 5-methyluridine (Mtu) in solution [2] by transient absorption spectroscopy with sub-30 fs temporal resolution [3]. The stimulated emission signal (Fig. 1) is directly related to the lifetime of the excited-state: For Urd the stimulated emission decays with a time constant of ca. 95 fs, whereas in MTU it shows a bi-exponential decay with a slower tail featuring a 2-ps time constant, suggesting that it involves a slower deactivation pathway of the $\pi\pi^*$ state. Our results, supported by simulations from first principles based on mixed quantum mechanics /molecular mechanics (QM/MM), allow us to identify ring puckering as the dominant deactivation channel and rationalize the difference in decay times with larger inertia of the methyl group in Mtu with respect to hydrogen in Urd.

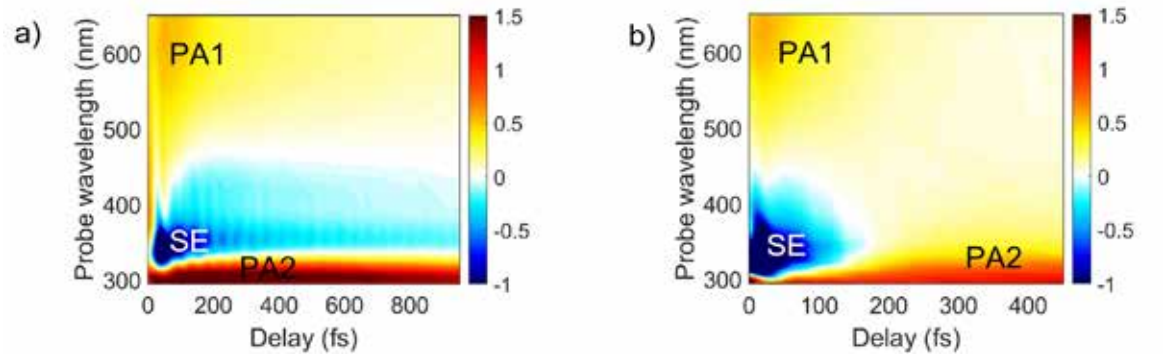

FIG. 1: Experimental pump-probe map of (a) 5-methyluridine and (b) uridine in solution (PA: photo-induced absorption; SE: stimulated emission).

Finally, I will present our progress towards the development of a pump-probe beamline combining UV and XUV pulses. Pulses as short as 10 fs or sub-5 fs in the UV range are demonstrated by non-linear upconversion [4] or dispersive wave emission in capillary fibers [5], being very promising for the investigation of electron dynamics in bio-relevant chromophores.

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All-XUV-Optical Nonlinear Absorption Spectroscopy with Free-Electron Lasers

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The optical response of matter to external radiation fields is intimately connected to the electronic structure and dynamics of the investigated system. In the linear regime, the interaction is well understood through Maxwell's classical description of light waves, and the response of the system is captured in the medium's refractive index, encoding both absorption and dispersion. Absorbing XUV and x-ray light, atom-specific inner-shell and core-shell transitions can be resonantly excited, providing a characteristic spectroscopic fingerprint of each system. Given the availability of short-wavelength free-electron lasers (FELs), delivering intense XUV and x-ray pulses at the femtosecond and attosecond timescale, new opportunities open up for the exploration of the nonlinear regime of light-matter interaction, with the ultimate goal to selectively steer the ultrafast quantum dynamics of matter at the fundamental electronic level inside atoms and molecules.

In this talk I will give an overview of our activities in the development of new concepts for nonlinear XUV-optical absorption spectroscopy with FEL light sources. We have built a versatile beamline for XUV-pump–XUV-probe transient absorption spectroscopy that was operated at the open-port beamline BL2 at the free-electron laser in Hamburg (FLASH) [1]. This has enabled the observation of XUV-intensity-induced modifications of the FEL absorption in atoms [2-7] which can be related to nonlinear interactions, including strong-coupling effects of resonant transitions. By identifying individual resonances in different molecular-fragment species, this technique also creates new opportunities for tracking site-specific molecular dynamics at an ultrafast timescale [8,9]. Last but not least, we have recently installed an XUV absorption spectroscopy beamline at the FLASH2 beamline FL26, which is equipped with a Reaction Microscope (REMI). The unique combination of the kinematically complete detection of electrons and ions after ionization in a REMI, with the sensitivity to bound-bound resonant transitions through absorption spectroscopy of the transmitted radiation, all driven by intense and ultrashort XUV-FEL pulses at FLASH2, opens new opportunities for fundamental nonlinear AMO science, and first results will be discussed in an outlook.

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A1-4-INV

Attosecond science at the Linac Coherent Light Source: recent developments and future directions

Agostino Marinelli (USA)

Stanford University - SLAC National Accelerator Laboratory

Free-electron lasers are the brightest sources of attosecond X-ray pulses, with a pulse energy that surpasses high-harmonic sources by more than six orders of magnitude.

In my talk I will present recent developments in attosecond science at the Linac Coherent Light Source. I will discuss the demonstration of attosecond soft X-ray pulses and the development of pump/probe techniques with sub-femtosecond temporal resolution. I will present the recent observation of coherent electron dynamics using angular streaking of Auger-Meitner electrons as well as X-ray pump/X-ray probe techniques. Finally I will present our plans for attosecond science at high-repetition rate with the LCLS-II superconducting accelerator.

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Interaction of trapped atoms with twisted light

Andrey Surzhykov[1,2], Anton Peshkov[1,2], and Yuriy Bidasyuk[1,2]

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Vortex (or twisted) light beams, that possess a helical phase front and carry nonzero projection of the orbital angular momentum (OAM) onto their propagation direction, attract currently considerable attention in many areas of modern physics. In particular, these beams were proven to be a valuable tool in microscopy, classical and quantum information transfer as well as for manipulation of microparticles and even Bose–Einstein condensates. During the recent years, moreover, a particular emphasis was placed also on the interaction of vortex light modes with single trapped atoms or ions. Several experiments have been performed, for example, to observe the operation of strongly forbidden atomic transitions by OAM photons [1,2]. Some of these transitions are discussed as candidates for novel frequency standards, and the use of the twisted light may ensure sufficient cancellation of the AC–Stark shift of their frequencies. In order to support the experiments on the interaction between vortex light and trapped atoms, we have recently developed theoretical approach that takes into account not only the time evolution of atomic population, exhibiting Rabi oscillations, but also excitation of the atomic center–of–mass degrees of freedom. We will illustrate the application of our theory for the particular cases of 4s $^2S_{1/2} \rightarrow$ 3d $^2D_{5/2}$ electric quadrupole transition in Ca^+ ion and $4f^{14}6s\ ^2S_{1/2}(F{=}0) \rightarrow 4f^{13}6s^2\ ^2F_{7/2}(F{=}3\ M_F = 0)$ electric octupole transition in Yb^+ ion. It will be discussed, in particular, how the topological charge and polarization of incident twisted light together with an orientation of the external magnetic field can be used to "tune" the probabilities and the AC–Stark shifts of these E2 and E3 transitions. Moreover, we will show how the Rabi oscillation dynamics can be affected by an interplay between an excitation of internal (atomic) and external (center–of–mass) degress of freedom.

The work was supported by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany's Excellence Strategy–EXC-2123 QuantumFrontiers–390837967.

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Probing charge-transfer neutralization reactions of atmospheric importance using the ion storage facility DESIREE

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The Double ElectroStatic Ion Ring ExpEriment (DESIREE) facility located at Stockholm University, Sweden, uniquely allows for studies of interactions between cations and anions at low and well-defined internal temperatures and centre-of-mass collision energies down to about 20 K and ~50 meV, respectively [1-3], and a schematic is shown in Figure 1.

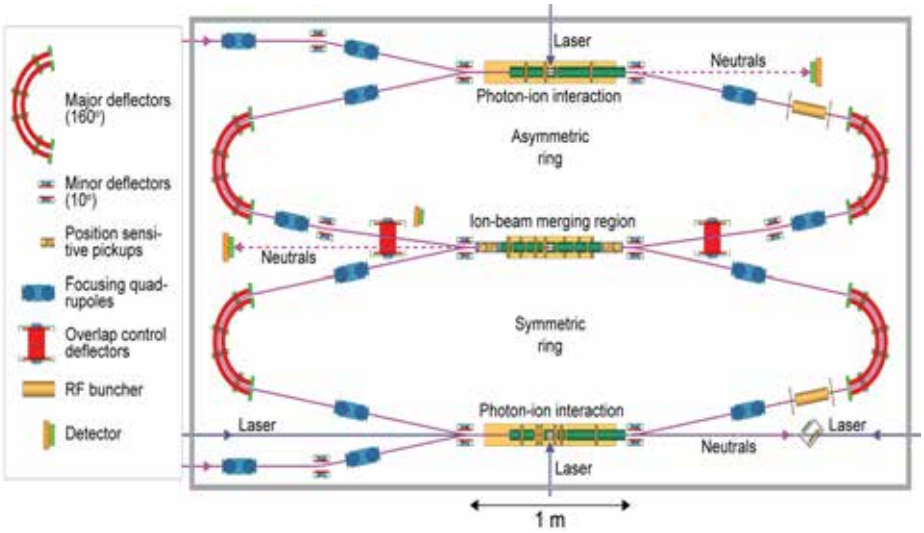

Figure 1: Schematic of the heart of the DESIREE facility: the two cryogenically cooled storage rings

Using this facility, we aim for a better understanding of how small and large molecules are formed and processed in astrophysical, atmospheric, and combustion plasmas, where we combine several novel experimental methods to build a fundamental understanding of the transfer of charge-, energy- and mass in collisional reactions. Control over the reaction environment [1-5] means that desired information, e.g., reaction products, can be obtained over many of the conditions needed to accurately model plasmas where these processes are important.

This talk highlights how this facility, which is the only one of its kind currently in the world, can play a crucial role in studying in mutual neutralisation reactions relevant to cool atmospheric plasmas, and I look at reactions involving atomic and molecular oxygen and nitrogen ions [4,5].

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This material is based upon work supported by the Air Force Office of Scientific Research under award number FA9550-19-1-7012.

Experimental Studies of Nonperturbative Dynamics in Heavy-Ion-Atom Collisions

P.-M. Hillenbrand[1,2], S. Hagmann[2], D. Banaś[3], E. P. Benis[4], C. Brandau[1,2], O. Forstner[2,5,6], J. Glorius[2], R. E. Grisenti[2], A. Gumberidze[2], M. O. Herdrich[5,6], M. Lestinsky[2], Yu. A. Litvinov[2], E. B. Menz[2,5,6], S. Nanos[4], N. Petridis[2], Ph. Pfäfflein[2,5,6], H. Rothard[7] M. S. Sanjari[2,8], U. Spillmann[2], S. Trotsenko[2], M. Vockert[5,6], G. Weber[6], Th. Stöhlker[2,5,6]

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Experimental data for atomic collisions of highly-charged ions are essential for benchmarking the theoretical description of dynamical processes in atomic physics. Of particular challenge is the accurate description of those processes that exceed the applicability of relativistic first-order perturbation theories. Recently, we have investigated two characteristic cases of such collision systems at the Experimental Storage Ring ESR of the GSI heavy-ion accelerator facility in Darmstadt, Germany:

(1) For fast collisions of U^{89+} projectiles with N_2 and Xe targets at 76 MeV/u, we studied the electron-loss-to-continuum cusp both experimentally and theoretically. We compared the continuum electron spectra of the two collision systems, which originate from the ionization of the projectile, and we were able to identify a clear signature for the nonperturbative character of the collision systems [1].

(2) For slow collisions of Xe^{54+} and Xe^{53+} with a Xe target at 30 and 15 MeV/u, we performed an x-ray spectroscopy experiment focusing on the target $K\alpha$ radiation. Experimental data for such slow symmetric collision systems are important for testing relativistic two-center calculations and provide an intermediate step towards understanding heavy-ion collisions in super-critical fields. We used the target $K\alpha$ satellite and hyper-satellite lines to derive cross-section ratios for double-to-single target K-shell vacancy production and compared our experimental results to theory applying a fully relativistic time-dependent two-center approach [2].

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Ultracold RbCs Molecules: Robust Storage Qubits And Rotationally Magic Traps

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Ultracold polar molecules offer many exciting opportunities in the fields of quantum computation, quantum simulation and fundamental studies of quantum matter. Many of these applications utilize the rotational states of the molecule and rely on long rotational coherence times. Achieving this in experiments has so far proved challenging, however, owing to the presence of large differential light shifts between rotational levels that result from the anisotropic molecular polarizability. We explore these light shifts using RbCs molecules confined in an optical trap. We use precision microwave spectroscopy of the rotational transition to probe the AC Stark shifts in the trap and reveal a rich energy structure with many avoided crossings between hyperfine states [1]. We show that hyperfine states in the rotational ground state may be used to engineer robust storage qubits in the molecules and using Ramsey interferometry demonstrate coherence times exceeding 5.6 s at the 95% confidence level [2]. We then show that similar coherence times should be achievable using a magic-wavelength optical lattice, where the polarizabilities are identical for two (or more) rotational states [3]. We report the development of such a magic trap at a wavelength of 1146nm. This wavelength lies between the $X^1\Sigma \rightarrow b^3\Pi$ vibronic transitions, allowing the anisotropic component of the polarizability to be tuned to zero. We present spectroscopy of the $X^1\Sigma \rightarrow b^3\Pi$ transitions and show that the differential shift of the N=0→N=1 rotational transition can be tuned to be zero in the magic trap for a detuning of approximately 175 GHz from the $X^1\Sigma(v=0,N=0) \rightarrow b^3\Pi(v'=0,N=1)$ transition. Finally, we will briefly describe ongoing experiments [4] to image and address single molecules in ordered arrays for applications in the field of quantum simulation.

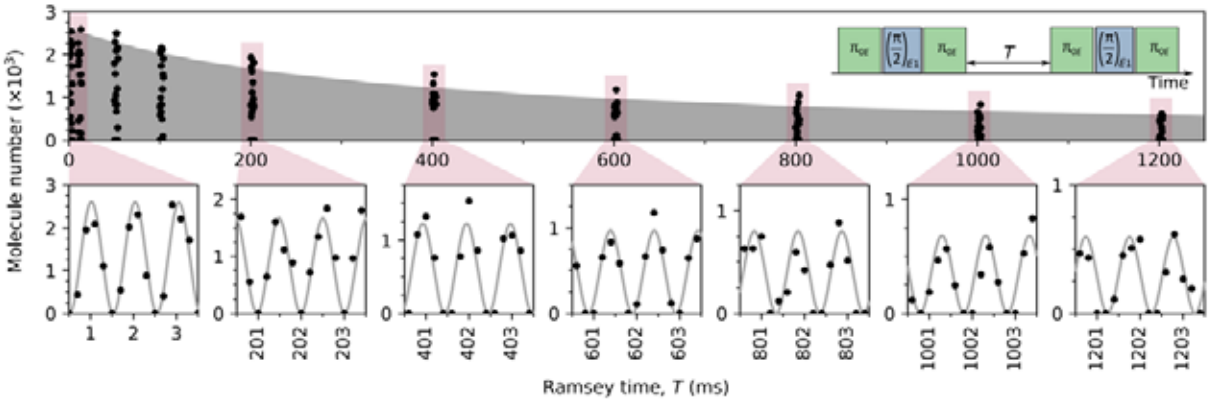

FIG. 1: Robust storage qubit in ultracold RbCs molecules showing long-lived coherence.

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Self-Pinning Transition of a Tonks-Girardeau Gas in a Bose-Einstein Condensate

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We show that a Tonks-Girardeau (TG) gas that is immersed in a Bose-Einstein condensate can undergo a transition to a crystal-like Mott state with regular spacing between the atoms without any externally imposed lattice potential. We characterize this phase transition as a function of the interspecies interaction and temperature of the TG gas, and show how it can be measured via accessible observables in cold atom experiments. We also develop an effective model that accurately describes the system in the pinned insulator state and which allows us to derive the critical temperature of the transition.

We will also show how extending the above idea to multicomponent TG gases can lead to the spontaneous emergence of more complex crystal structures with antiferromagnetic order, and how finite interactions in the immersed component lead to additional superfluid phases.

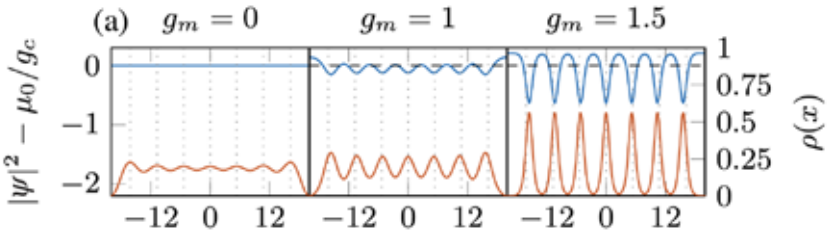

Figure 1: TG gas density $\rho(x)$ (red lines) and BEC depletion (blue lines) for $N = 7$ TG atoms and increasing interaction strengths g_m between the two components. The pinning of the TG gas component in the self-created matter wave lattice for larger g_m is clearly visible..

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A Weakly-Interacting Many-Body System of Rydberg Polaritons based on Electromagnetically Induced Transparency

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We proposed utilizing a medium with a high optical depth (OD) and a Rydberg state of low principal quantum number, *n*, to create a weakly-interacting many-body system of Rydberg polaritons, based on the effect of electromagnetically induced transparency (EIT). The Rydberg polaritons are the quasi-particles representing superpositions of photons and Rydberg coherences. We experimentally verified the mean field approach to weakly-interacting Rydberg polaritons, and observed the phase shift and attenuation induced by the dipole-dipole interaction (DDI) [1,2]. The measured DDI-induced phase shift and attenuation are consistent with the theoretical predictions, and can be viewed as a consequence of the elastic or inelastic collisions among the Rydberg polaritons. Using this weakly-interacting system, we varied the DDI strength via the input photon flux and measured the transverse momentum distribution of the Rydberg polaritons. We further showed that a larger DDI strength caused the width of the transverse momentum distribution of Rydberg polaritons to become smaller as shown in Fig. 1, indicating that the thermalization process was driven by the elastic collisions [2]. The experimental data reveal that the effective transverse temperature was reduced from 3.1 μK to 1.2 μK during the propagation of Rydberg polaritons through the medium. The combination of the μs-long interaction time due to the high-OD EIT medium and the μm^2-size collision cross section due to the DDI suggests a new and feasible platform for the Bose-Einstein condensation of weakly-interacting Rydberg polaritons.

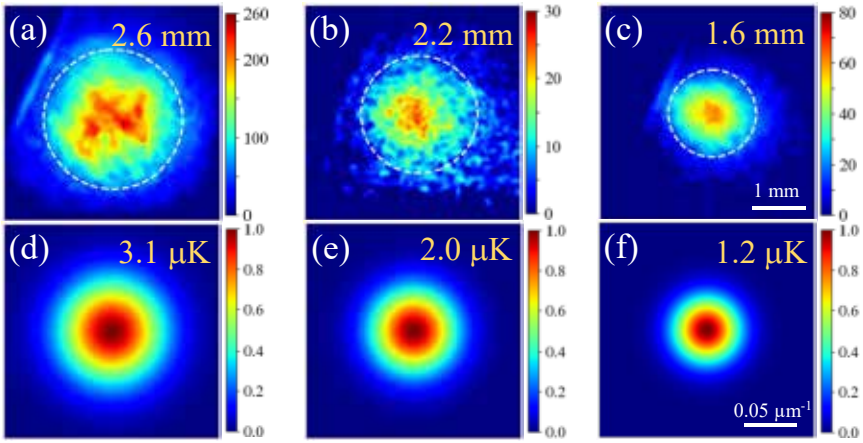

FIG. 1: (a-c) Time-of-flight images of photon distribution profile. (d-e) The corresponding momentum distributions of Rydberg polaritons.

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Response of Small Helium Clusters to Strong Laser Fields

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Small helium clusters are peculiar few body quantum systems. The helium dimer has a single weakly bound state of a huge spatial extent. About 80% of its probability distribution resides in the classically forbidden tunnelling region [1]. This is why such objects are termed "quantum halos". The helium trimer has two bound states, one of which is of Efimov nature [2]. We have utilized Coulomb explosion imaging implemented within a COLTRIMS reaction microscope for measuring spatial probability distributions of these quantum systems.

Recently we have combined Coulomb explosion imaging with the pump-probe approach for studying field-induced dynamics in small helium clusters. A strong laser field of the pump pulse tunes the interaction between helium atoms in a dimer brining about its dissociation. The dissociating wave packet has been imaged by the probe pulse that triggers the Coulomb explosion of the cluster. Due to the interference with the giant ground state wave function, not only the amplitude of the dissociating wave packet, but also its quantum mechanical phase has been observed (FIG. 1) [3].

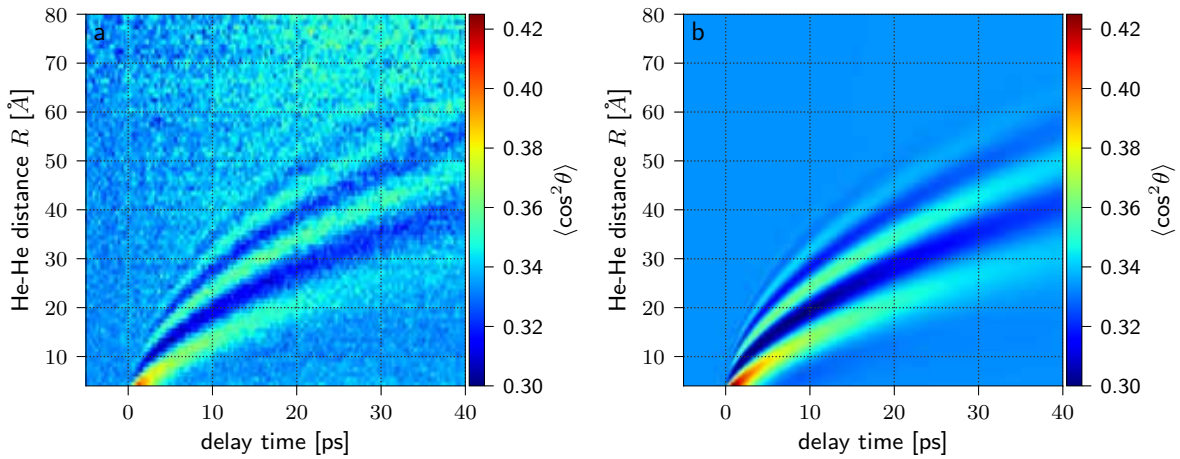

FIG. 1: Temporal evolution of the field-induced alignment of $^4He_2$ [3]. a) - experiment, b) - theory. The expectation value of $\cos^2\theta$ is coded with color. θ is an angle between the dimer axis and the direction of laser polarization.

Preliminary results on the field-induced dynamics of helium trimer indicate its partial dissociation. The further details about the temporal response of these two clusters to strong laser fields is going to be discussed.

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Absolute Measurement of a THz Transition Frequency Referenced to a Magnetic Dipolar Transition in Ca^+ ion

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A three-photon Coherent Population Trapping [1] is observed by the dark line it induces on the laser induced fluorescence of a laser-cooled Ca^+ ion cloud. This dark line is referenced to a magnetic dipolar transition at 1.8 THz, between two fine-structure sub-state of the metastable *D*-state. We explore the performance of such a system for frequency metrology in the THz domain[2]. To that purpose, the three involved lasers are made phase coherent thanks to a phase-lock on the same optical frequency comb (OFC)[3], that is locked on an ultra-stable laser, a home-made Ti:Sa laser (see FIG. 1). The absolute measurements of this transition frequency is made possible through the comparison with an ultra-stable optical signal referenced to the SI second and delivered by an optical fibre link (the REFIMEVE+ signal). The uncertainty in the measured frequencies is of the order of 100 Hz, limited by the experimental line-width which can reach 10 kHz. Comparison with the best known value for this transition frequency [4] shows shifts of the order of kHz that will be discussed.

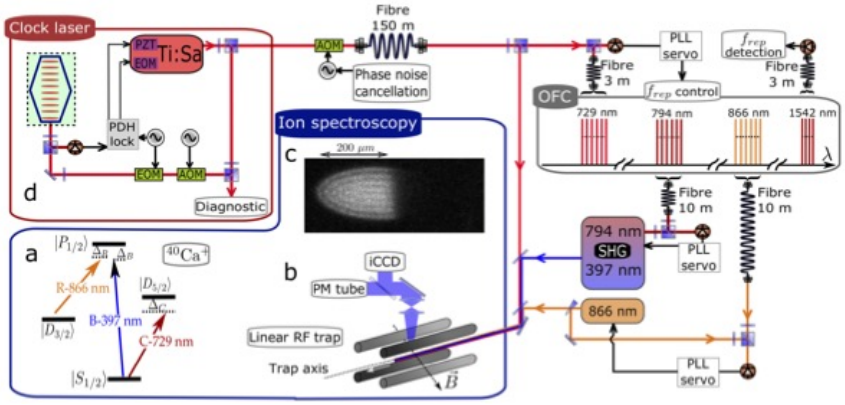

FIG. 1: **a** : transition scheme for 3 photons-CPT in Ca^+, **b** : experimental set-up **c** : picture of an ion cloud made of 710 (±35) ions, the dark ions are separated from the bright ones by the radiation pressure induced by laser cooling. **d**: phase lock-in set-up, involving an OFC and an ultra-stable laser.AOM : acousto-optic modulator, EOM : electro-optic modulator, PDH : Pound-Drever-Hall, PLL : phase-lock loop, SHG : second harmonic generation.

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Extending coherent multidimensional spectroscopy to new target systems and new light sources

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Coherent multidimensional spectroscopy (CMDS) is a powerful ultrafast spectroscopy technique which reveals couplings and system-bath interactions with unprecedented detail. While CMDS is mainly applied to liquid phase samples, we have recently extended the method to cluster beams prepared in the gas phase [1,2]. In contrast to experiments in the condensed phase, cluster beams provide isolated nanosystems in which fundamental molecular processes can be studied with high resolution. Furthermore, we have implemented wave packet interferometry, the basic principle of CMDS, with new extreme ultraviolet light sources [3,4]. This opens up the perspective of CMDS experiments with attosecond time resolution and element specific probing.

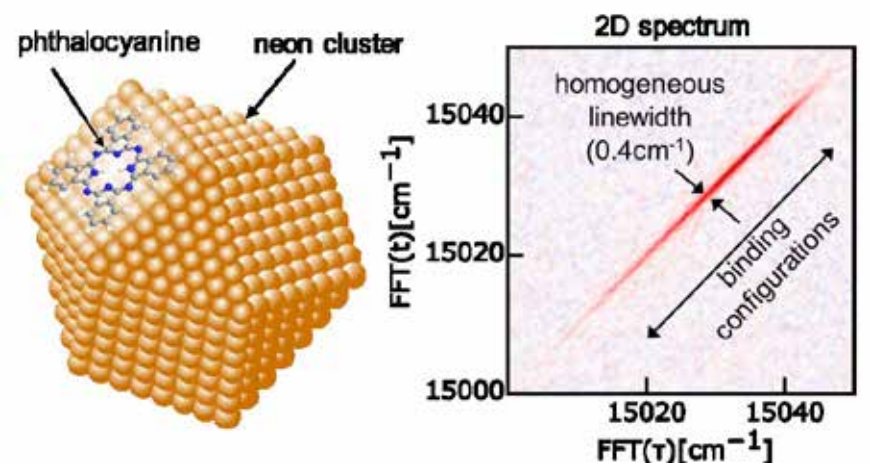

FIG. 1: High-resolution 2D spectrum of free-base phthalocyanine molecules attached to a neon nanocluster in the gas phase. CMDS directly separates the homogeneous and inhomogeneous lineshapes from which information about the binding configurations with the nanocluster environment can be gained.

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Terahertz Frequency

Luigi Consolino

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High precision THz spectroscopy of rotational and ro-vibrational molecular transitions promises to deliver many novel physical insights. In order to fully exploit the potential of this key spectral region, the challenge is to merge, in a single source, three crucial aspects: a broad spectral coverage, metrological-grade performances (i.e. high resolution and accuracy with referencing to the primary frequency standard), power levels sufficient for room-temperature detection. In this framework we will report on two different approaches for THz metrological-grade radiation, the first related to difference frequency generation (DFG) based broadband continuous wave (CW) THz source, the second regarding the characterization and applications of Quantum Cascade Lasers (QCL) based THz frequency combs (FCs).

1. DFG-based broadband CW THz source

In our work, we demonstrate room-temperature generation and detection of continuous-wave THz radiation spanning three octaves in the THz range, from 1 to 7.5 THz, and performing high-accuracy molecular spectroscopy. This unprecedented result makes use of a simple, reliable approach that combines, in a unique set-up, robust telecom laser components with difference-frequency nonlinear generation.

The main contribution of our work is the combination of all the following aspects: i) room temperature CW generation, based on the fully-developed and commercial telecom fiber laser technology that grants a high level of compactness, stability and reliability to our new source; ii) a 3-octave spectral coverage, from 0.97 to 7.5 THz, that is obtained by the combined use of a Cherenkov emission scheme and strong light confinement in a surface nonlinear waveguide; iii) high power levels enabling both room temperature detection and high-precision THz spectroscopy, achieved thanks to a CW generation efficiency as high as 10^{-7} W^{-1} ; iv) frequency referencing to the primary frequency standard by means of a mode-locked femtosecond laser and a GPS disciplined Rubidium-Quartz oscillator; v) a state-of-the-art accuracy in the order of 10^{-9} obtained with a room temperature Golay cell detector. The proposed approach paves the way to a new class of metrological-grade sources spanning most of the THz range for countless demanding applications.

2. QCL-based THz frequency combs

Quantum Cascade Lasers (QCLs) technology, both in the mid-infrared and THz region, is exploiting the extraordinary versatility of these devices for developing active regions with engineered optical dispersion that emit optical frequency combs. Thanks to four-wave-mixing non-linear processes happening inside the active medium, proper mode-locking is obtained. The Fourier modal phases, ultimately describing comb operation are retrieved thanks to the Fourier Analysis of Comb Emission (FACE) technique, which confirms the high level of coherence of these sources, and enables retrieval of the temporal emission profile.

The metrological-grade performance of this class of devices is probed thanks to the full phase referencing to the primary frequency standard, achieving ~2 Hz in 1 s stability and ~6 Hz accuracy for the emitted modes. Independent and full control of the two comb degree of freedom is also demonstrated and characterized. Finally, application of a QCL-FC to high-accuracy molecular spectroscopy is shown in a hydrid dual comb spectroscopy (DCS) setup. The most distinctive characteristic of this approach is the merging of two completely different comb in a dual comb spectrometer. This allows merging the high power per mode emitted by the QCL device with the accuracy and frequency referencing allowed by an optically rectified free-standing THz FC.

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, $|J_{K_a K_c}\rangle = |0_{00}\rangle$. Details of the experimental scheme as well as results will be discussed in the presentation.

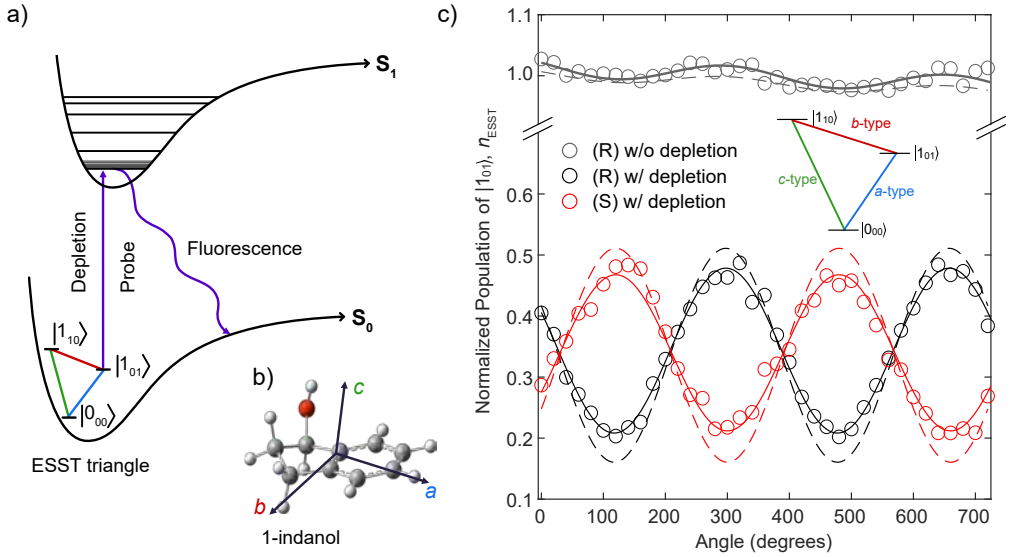

FIG. 1: (a) The energy level scheme illustrates the electronic excitation, depletion and probe, from the rotational state $|1_{01}\rangle$ of ESST triangle, and emission process used for detection. (b) The most stable conformer of 1-indanol with its inertial axis. (c) The population of the target state $|1_{01}\rangle$ as a function of the phase of the b-type microwave field normalized to its original thermal population. ESST results with depletion for (R)- and (S)-enantiomers are marked in black and red circles, the fit as a solid line, and the theoretical prediction as a dashed line, adapted from [4].

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K-LL Auger Decay of Doubly Excited States of Argon

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Numerous high-resolution spectroscopic studies of decay products of singly-excited core-hole atomic states $A(C^{-1}V)$ show that signal broadening originates in the combined experimental resolution and natural broadening of the final state. Although the core-hole lifetime significantly broadens photoabsorption and photoelectron spectra, this contribution is entirely absent due to the energy conservation when ω' photons and e_{RA} electrons are observed in the resonant inelastic x-ray scattering $\omega + A \rightarrow A(C^{-1}V) \rightarrow A(V'^{-1}V) + \omega'$ and the photoinduced resonant Auger decay $\omega + A \rightarrow A(C^{-1}V) \rightarrow A^{+}(V'^{-2}V) + e_{RA}$, respectively. From RIXS and RA yields, recorded by the ω probe covering the C^{-1} photoabsorption edge and with ω' and e_{RA} scanning the characteristic fluorescence and Auger electron spectral region, respectively, the absorption spectra with "subnatural" resolution were extracted giving rise to new details about valence excitations (HERFD and HEROS techniques). Moreover, the competing decay channels, such as ultrafast molecular dissociation and charge transfer were characterized by studying nonlinear dispersion of the characteristic lines in 2D maps of decay products.

Sharp experimental energy resolution and energy shift of satellite x-ray lines also enabled separation of RIXS signal of $(CV')^{-1}V^2$ doubly excited states and the asymptotic $A^{+}(CV')^{-1}V$ shake-up and $A^{2+}(CV')^{-1}$ shake-off channels from the underlying C^{-1} ionization continuum [M. Kavčič et al, Phys. Rev. Lett. 102, 143001 (2009)]. We have now measured 2D maps pertaining to K-LL RA decay of $(1s3p)^{-1}nln'l'$ doubly excited states in argon. The difference with our previous K_β RIXS map of the same states is that electron spectrometer at GALAXIES beamline at SOLEIL synchrotron achieves better spectral resolution (0.4 eV at 2650 KE) than x-ray spectrometer (0.6 eV at 3190 eV) but at the same time, the broadening of final RA states with two $2p$ vacancies is quite significant (0.3 eV) and can not be neglected. Nevertheless, since different doubly excited states can generate Auger electrons with substantially different kinetic energies, it is now possible to isolate from RA map the contributions of separate (groups of) resonances to the absorption spectrum. This is hardly achievable with the RIXS measurement because the characteristic x-ray yield peaks at about the same emission energy for all resonant states and the multiplet splitting of final states is smaller. The new data is compared to the calculated K-LL RA maps of doubly excited states in argon where effects of interference of the neighboring absorption-emission paths are taken into account together with angular selectivity of the actual experiment.

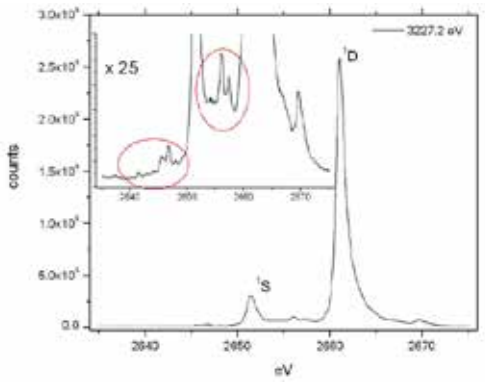

Figure 1: K-LL resonant Auger spectrum of $Ar(1s3p)^{-1}nln'l'$ states superimposed on K-LL spectrum of the single core hole state $Ar^{+}1s^{-1}$. Resonant excitation gives a maximum yield at $\omega = 3227.2$ eV.

A3-1-INV

Molecular polaritonics and subwavelength cavity QED

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Universidad Autónoma de Madrid

When the interaction of molecular excitations with quantized light modes becomes sufficiently strong, the strong-coupling regime is entered and the eigenstates of the system become hybrid light-matter excitations, so-called polaritons. In wavelength-scale optical cavities, polaritons are delocalized states that arise due to the collective interaction of macroscopic numbers of molecules with the same light mode and thus have fundamentally different characteristics than the single-molecule excitations that they are formed from. Polariton formation thus provides a control knob that can be used to affect a number of material properties without having to modify the material itself. I will discuss several examples of such effects, including changes of the absorption and emission characteristics of a material, of energy transfer between molecular species, and even of photochemical reactions. I will then discuss situations in which plasmonic nanocavities are used to confine light to strongly subwavelength dimensions, increasing the light-matter interaction sufficiently that the strong-coupling regime can be reached with just one or a few molecules. In these cases, the energy level structure and dynamics of the molecule are affected even more strongly than in the collective case. Additionally, ultrafast losses are unavoidable in such cavities, leading to additional loss-induced effects. I will discuss several strategies to not only mitigate but exploit these fast losses.

New Perspectives on Quantum Geometry, Superconductivity and Bose-Einstein Condensation

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Superconductivity, superfluidity and Bose-Einstein condensation (BEC) are many-body phenomena where quantum statistics are crucial and the effect of interactions may be intriguing. Superconductors are already widely applied, but theoretical understanding of superconductivity and condensation in several real-world systems is still a challenge, and superconductivity at room temperature remains a grand goal. We have discovered that superconductivity (superfluidity) has a connection to quantum geometry [1]. Namely, the superfluid weight in a multiband system has a previously unnoticed component which we call the geometric contribution. It is proportional to the quantum metric of the band. Quantum metric is connected to the Berry curvature, and this allows to relate superconductivity with the topological properties of the band. Using this theory, we have shown that superconductivity is possible also in a flat band where individual electrons would not move. Recently, we and other groups have shown [2,3] that these results are essential in explaining the intriguing observation of superconductivity in bilayer graphene and may eventually help realize superconductors at elevated temperatures. We have also explored the effect of quantum geometry on Bose-Einstein condensation [4].

Bose-Einstein condensation has been realized for various particles or quasi-particles, such as atoms, molecules, photons, magnons and semiconductor exciton polaritons. We have experimentally realized a new type of condensate: a BEC of hybrids of surface plasmons and light in a nanoparticle array [5]. The condensate forms at room temperature and shows ultrafast dynamics, and the system provides easy tunability of the lattice and unit cell geometry and symmetries. Recently, we have observed formation of polarization textures and domain walls, and obtained the BEC phase for the first time using a phase retrieval algorithm [6]. Our measurements of spatial and temporal coherence show a change from exponential decay to power-law when crossing to the BEC phase [7]. We have also observed that when the nanoparticles are made of magnetic material, chiral modes and magnetic switching of lasing become possible [8]. This paves the way for future studies of topological effects in these systems.

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Quantum light-induced nonadiabaticity in molecular systems

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Abstract

The interaction of a molecule with the quantized electromagnetic field of an optical or plasmonic nanocavity gives rise to polaritonic (hybrid light-matter) states and light-induced conical intersections (LICI) between polaritonic potential energy surfaces. In LICI situation the vibrational, electronic and photonic modes of the system are coupled nonadiabatically providing extremely large nonadiabatic coupling (NAC) at the degeneracy point. Due to this strong coupling the Born-Oppenheimer approximation (BOA) loses its validity resulting in remarkable changes in the different dynamical, spectroscopic and topological properties of the molecular systems. During the talk, results are presented to demonstrate the spectroscopic as well as the dynamical fingerprint of the LICI in a polyatomic molecule. First, we investigate the validity of the BOA, neglecting nonadiabatic coupling between polaritonic surfaces, in relation to spectroscopy. We show that the BOA may fail even if one vibrational degree of freedom is treated and generally fails for two- or more-dimensional vibrational models due to LICI by the cavity [1]. Second, we demonstrate that the time-resolved ultrafast radiative emission of the cavity enables to follow both nuclear wavepacket dynamics on and nonadiabatic population transfer between polaritonic potential energy surfaces. The latter provides an unambiguous (and in principle experimentally accessible) dynamical fingerprint of the LICI [2].

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A fresh perspective on the Casimir effect

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The Casimir effect [**1**, **2**], which predicts the emergence of an attractive force between two parallel, highly reflecting plates in vacuum, plays a vital role in various fields of physics, from quantum field theory and cosmology to nanophotonics and condensed matter physics. Nevertheless, Casimir forces still lack an intuitive explanation and current derivations rely on regularisation procedures to remove infinities. Moreover, their standard derivation simply assumes that mirrors restrict the field inside the cavity to standing waves with a discrete set of frequencies. However, standing wave mode models cannot take into account from which direction light enters an optical cavity and therefore cannot reproduce the typical behaviour of Fabry-Perot cavities [**3**]. Discrete mode models also imply that no light is permitted inside a cavity with mirror distances well below typical optical wavelengths, which contradicts recent nanocavity experiments [**4**]. An alternative approach is needed.

Starting from special relativity and treating space and time coordinates equivalently, we overcome no-go theorems of quantum electrodynamics and obtain a local relativistic quantum description of the electromagnetic field in free space [**5**, **6**, **7**]. When extended to cavities, our approach can be used to calculate Casimir forces directly in position space without the introduction of cut-off frequencies. Our local relativistic description provides additional insight by attributing Casimir forces to a certain change of the topology of the quantised electromagnetic field inside the cavity (cf. Fig. 1).

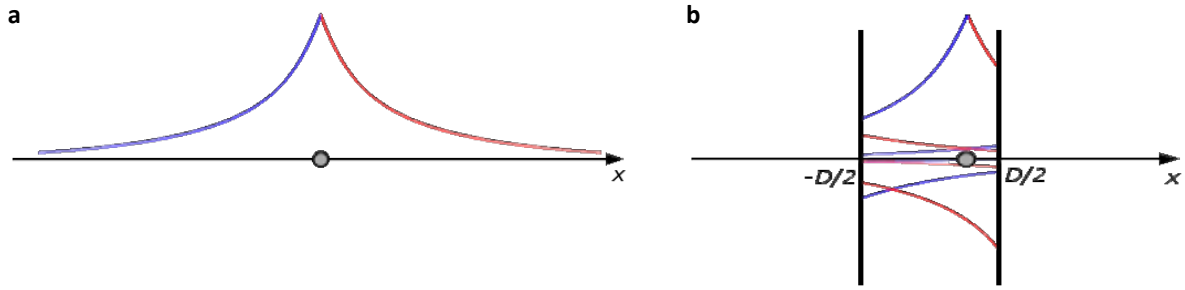

FIG. 1: **a.** Local blip excitations contribute to local electric and magnetic field expectation values everywhere along the x axis. **b.** Since a blip on one side of a highly reflecting mirror cannot contribute to the field expectation value on the other side, its field contribution must be folded back on itself. This effect alters the electric and magnetic field observables in the presence of a mirror and leads to interference effects which are at the origin of Casimir forces.

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Spectroscopy of helium-tagged molecular ions

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Helium nanodroplets (HNDs) are very versatile cryogenic flying nanoreactors with outstanding properties allowing the isolation of diverse molecular ions and the formation of clusters at sub-Kelvin temperature. The conditions inside HNDs are ideal to study chemical reactions and to perform spectroscopic studies of the dopant ions.
In this contribution, we will present a newly developed setup which combines several experimental techniques and methods, evolved and tested in the last years.
One of these techniques is the formation of highly charged HNDs by electron impact [1]. In dependence of the electron energy, positively or negatively charged HNDs are formed. The charges are distributed across the droplet surface and attract the dopants, which are picked-up by the traversing beam of HNDs, and are ionized by charge transfer processes [2]. The formation of several nucleation sites in a single HND enables the production of intense beams of cold dopant ions.
The release of the latter from the HND environment or the formation of dopant ions decorated with a few He-atoms, respectively, is achieved by 'splashing' the doped HNDs onto a surface [3] or by gentle shrinking of the helium matrix due to collisions with helium gas at room temperature [4]. The latter technique is used in the new setup. The ions gained by using these methods are perfectly suitable to be studied by laser spectroscopy in combination with a time-of-flight mass-spectrometer.
In contrast to previous studies, where the absorption spectra are predominantly obtained from the precursor ion depletion, the new setup enables the detection of the photoproduct from virtually zero background signal. This enables high quality spectra even for weak absorption lines at reduced data acquisition times. Recent results obtained with the new setup will be presented.

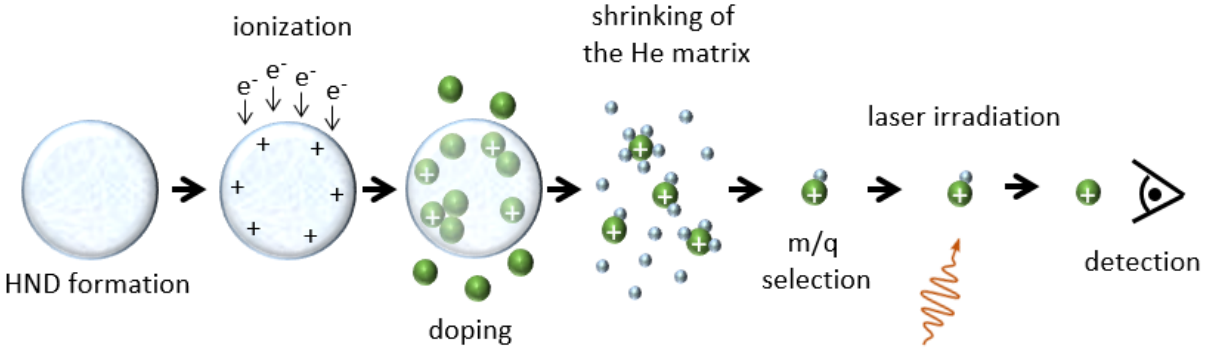

FIG. 1: Schematic of the formation of helium-tagged and mass-per-charge selected (cluster) ions for performing messenger-type laser spectroscopy in combination with a time-of-flight mass-spectrometer.

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Environmental Effects on Electron Attachment

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We experimentally probe interaction of low energy electrons (<10eV) with isolated molecules and clusters. These experiments enable us to explore effects of various environments on the electron attachment (EA).

Latterly, we primarily focus on electron attachment in radiation chemistry of living tissue, exploring DNA components and radio-sensitizing pharmaceuticals. Isolated DNA bases undergo hydrogen loss via dissociative electron attachment forming typical $(M\text{-}H)^-$ DNA base radical anions. In our study [1], we demonstrated closing of this dissociation channel by the water environment. On another model system, radio-sensitizer nimorazole, we demonstrated that while the resonance position in the water remains unchanged, the dissociative resonances changes to associative.[2] Therefore, the closing of dissociation channels upon EA is mainly caused by caging of the dissociation products and intermolecular energy transfer [3]. In more complex biomolecules such as the nucleotides, negative ions formed upon EA can accept hydrogen from the surrounding environment, which can dramatically change the fragmentation and final charge redistribution over the molecule and fragments. [4] Finally, e.g. radiosensitizer misonidazole, we have shown that environment can also lower the dissociation barriers [5].

Interesting environmental effects could be observed also for molecules of technological interest. In butadiene, we observed effective intermolecular vibrational energy redistribution stabilizing the butadiene cluster anions and giving us a novel view of charge accommodation by dielectric clusters and nanoparticles [6]. In thiophenols, with EA being the first step in their plasmon mediated chemistry [7], we observed a dissociation mechanism dependent on the molecule hydration site [8]. The present talk will highlight the most important experimentally observed effects of the environment on electron attachment.

I acknowledge the support by European Regional Development Fund; OP RDE; Project “CARAT” no. CZ.02.1.01/0.0/0.0/16_026/0008382.

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Charge migration in betaine by impact of fast atomic ions

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Following the ionisation, the very early stages of radiation matter interaction are characterised by charge migration within the molecular edifice mostly governed by electronic dynamics. From an experimental point of view, it is necessary to have access to femtosecond timescales.

The advent of fs-resolved pump-probe scheme using high order harmonics generation laser or free electron lasers allows to suddenly ionise with the pump beam the system and to probe its dynamics using the probe beam. Alternatively using X-ray ionisation, Auger decay and Coulomb explosion also allow to clock the dynamics. Ion collisions are also characterised by a fs timescale excitation of matter, but contrary to photoionisation they are less selective, moreover there is no pump-probe scheme available on fs timescale using conventional ion accelerators.

Here we exploit the zwitteronic nature of the betaine molecule to induce a double electron capture from the negatively charged carboxylate group of the molecule in the collision with a low-energy O^{6+} ion. This results in the formation of a molecular dication with two charges localised to both ends.

Beside the expected charge separation giving two charged fragments associated with both ends, we observe ion-pairs resulting from the dissociation of doubly charged ends and thus associated with a charge migration following the ionisation.

Nonadiabatic molecular dynamics calculations show that the electronic dynamics associated with charge migration occurs in the ground state of the betaine dication. It is efficiently populated in ion collisions by the resonant double electron capture.

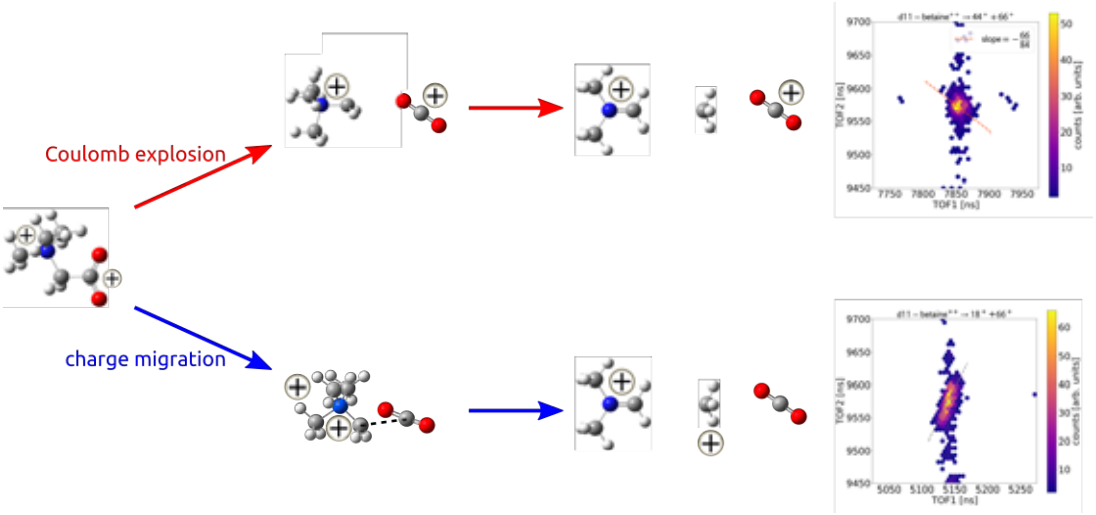

FIG. 1: Competition between Coulomb explosion and charge migration in the dissociation of betaine dication produced in collision with 48 keV O^{6+} ions.

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Ultrafast Processes in Amino-Acids, Amino-Acids Derivatives and Clusters of Amino-Acids Induced by Ionizing Radiation

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Biomolecules exposed to ionizing radiation can undergo numerous complex process, such as isomerization and roaming, leading to changes in their molecular and electronic structure. In the last years, we have studied the fragmentation dynamics induced by collisions with highly-charged ions in amino-acids and amino-acids derivatives. When these molecules are ionized and excited in the collisions, they follow the so-called Coulomb explosion, where the charge splits in different fragments that repeal each other after cleavage of bonds in the molecular backbone. However, other non-expected processes appear in competition, such as hydrogen migration. They occur in the cation and dication molecules, and take place within a few tens of femtoseconds to picoseconds [1,2]. We have also determined the distribution of the energy deposited in the ionized molecule as a result of the collision [3], which is the responsible for triggering the atomic reorganization.

The formation of peptide bonds by energetic processing of amino-acids is an important step towards the synthesis of biologically relevant molecules and, in this context, we have also studied the formation of peptide bonds in single collisions of low-energy He^{2+} ions (α-particles) with loosely bound clusters of β-alanine molecules [4].

Light irradiation of biomolecules produces ionization and can also initiate interesting physicochemical processes. We have recently shown [5] that VUV radiation with cyclic amino-acids, in particular cyclo-(alanine-alanine) one of the 2,5-diketopiperazines (DKPs), generates reactive oxazolidinone intermediates; the interaction of these intermediates with other neutral and charged fragments, released in the molecular decomposition, leads either to the reconstruction of the cyclic dipeptide or to the formation of longer linear peptide chains. These results explain how DKPs can survive hostile chemical environments as well as provide the seed for amino-acid polymerization.

A complete picture of the mechanisms underlying the different dynamics were obtained using both experimental and theoretical state-of-the-art techniques. The experiments combine molecular irradiation, either with highly-charged ions or with energetic photons, and coincident detection of the produced particles, with ion-ion coincidence mass spectrometry or with photoelectron-photoion coincidence (PEPICO) measurements. Simulations were performed with quantum chemistry methods: ab initio molecular dynamics and density functional theory calculations.

In this communication, comparison of the dynamics and mechanisms of the different processes induced in the ionizing radiation observed in the above-mentioned biomolecules, will be presented and discussed.

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High Resolution Resonant Auger Spectroscopy of Ultrafast-decaying Core-ionized Atoms

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Highly intense X-ray pulses from X-ray free-electron lasers (XFELs) allow studying non-linear photo-induced processes in atoms and molecules in the short wavelength regime. These can include sequential and non-sequential multiphoton ionization and excitation processes. Sequential ionization processes induced by X-rays involve core-shells and occur in competition with ultrafast relaxation via Auger emission or fluorescence. When the X-ray intensity is high enough, this competition becomes effective and the population of transient highly excited ions exposed to the radiation becomes significant, so that a spectroscopic characterization of the ultrashort-lived states is made possible.

By using the intense pulses from the SASE3 soft X-ray undulators at European XFEL, we studied the core-hole excitation of transient, highly excited ions by means of resonant Auger electron spectroscopy employing the Small Quantum Systems (SQS) instrument. Neon was ionized at the 1s shell and, depending on the photon energy, either sequentially ionized to Ne^{2+} $1s^02s^22p^6$ or excited to different Ne^{+*} $1s^02s^22p^6np$ Rydberg states within the same fs X-ray pulse. The first study [1] was performed with relatively low photon energy resolution using the unmonochromatized beam from the undulator. We scanned the photon energy across the $1s^12s^22p^6 \rightarrow 1s^02s^22p^6np$ resonances with steps of 1 eV (much smaller than the FEL bandwidth of about 8.5 eV). The resulting Auger electron spectra were recorded by electron time-of-flight spectrometers (eToFs). The selective excitation of different Rydberg states was limited by the bandwidth of the X-ray pulses.

We have recently been able to perform the same study using the beam delivered by the SASE3 monochromator, with a bandwidth as low as 300meV. This allowed us to study the ultrafast-decaying core-ionized Ne atoms with unprecedented spectroscopic resolution for non-linear studies, selectively exciting the different states and measuring the decay into the final states populated by resonant Auger electron decay. Using three eToFs looking at the interaction region under different angles, we could measure the angular anisotropy of the resonant Auger electrons. The comparison of the measurements with the recently published theoretical results [2] allowed a quantitative insight into the angular anisotropy of the different final states as well as into the role that shake-up processes play in their formation. These results are benchmarking the performance of the SQS instrument at European XFEL and demonstrate the novel possibilities which have been opened up in particular for investigations of non-linear phenomena and ultrafast decaying transient states in atoms and molecules in the X-ray domain.

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Attosecond Science at the FERMI Free Electron Laser

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Temporal coherence is one of the quintessential properties of lasers, and its applications at optical wavelengths are ubiquitous. There is a strong drive towards extending the same techniques to shorter wavelengths, due to their ability to more directly access the motion of electrons in atoms and molecules, as well as their ability to access core orbitals, with chemical sensitivity.

Free-Electron-Lasers (FELs) in the EUV and XUV photon energy range have greatly expanded the feasibility range of experiments at the crossroad between tabletop lasers and synchrotrons, but the mechanism responsible for radiation emission (self-amplified spontaneous emission, SASE) causes them to lack temporal coherence.

The FERMI facility in Trieste (Italy) is unique in the FELs landscape because it has been designed as a seeded source, resulting in superior performance in terms of control and reproducibility of its light pulses [1]. Transverse and temporal coherence are those expected from a true laser, and have been exploited in a series of pioneering experiments; the possibility of accommodating more than one seed pulse, and the modular layout of the radiating undulators provide the opportunity of generating phase-locked harmonics, with full independent control of their amplitude and relative phase, or twin phase-locked pulses. In all cases, the phase accuracy is well below the periodicity of the radiation, and corresponds to sub-attosecond intervals.

Demonstrated applications range from the coherent control of a photoionization process [2], to the measurement of photoemission delays [3], the use of phase as a reference for increased sensitivity [4], or the generation of periodic waveforms [5]. The experiments that will be presented have been performed at the Low Density Matter (LDM) beamline at FERMI, serving the atomic, molecular and cluster science community since its opening at the end of 2012 [6]. The results originate from the joint effort of many international laboratories and of a large number of researchers, whose work is gratefully acknowledged.

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Two-Color X-Ray Pump-Probe Spectroscopy at SwissFEL

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The soft X-ray branch Athos at SwissFEL [**1**] has been designed to produce intense few to sub-fs soft X-ray pulses (250 eV to 1800 eV) with multiple colors. The Maloja endstation has been tailored to make ideal use of these special beam modes by providing a flexible platform to combine multiple experimental techniques and to enable new experiment geometries. The unique combination of Athos and Maloja allows to investigate a large range of phenomena in the field of atomic, molecular, non-linear and chemical sciences ranging from ultrafast dynamics to non-linear X-ray sciences. During this talk, I am going to present first results from the endstation commissioning and the pilot experiment phase.

Multi-color X-ray pulses with adjustable delay allow to follow ultrafast charge and energy transfer in time and space due to the state selectivity of X-ray photoabsorption. With two freely tunable X-ray pump-probe energies from the Athos line [**2**], we can excite at one atomic site and monitor subsequent relaxation processes throughout a system at another site. In this talk, I will show results from our first two-color experiment on small gas-phase molecules. We employed transient absorption spectroscopy to track the core-excitation induced dynamics in nitrous oxide by exciting the molecules with a pump pulse tuned to the nitrogen K-edge and probing with a pulse tuned to the oxygen K-edge. Pushing the pulse duration into the few to sub-fs regime will give access to study X-ray induced dynamics on sub-Auger lifetimes. This is crucial to understand processes like charge migration or the initial steps of radiation damage, and to implement nonlinear X-ray spectroscopy techniques.

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Anisotropic dynamics of two-photon ionization: real time imaging of photoemission

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Imaging in real time the complete dynamics of a process as fundamental as photoemission has long been out of reach due to the difficulty of combining attosecond temporal resolution with fine spectral and angular resolutions. To achieve this, a key ingredient is the relative phase between the spectral components of the photoionized wavepacket, that can be measured using interferometric schemes such as the RABBIT technique [**Paul2001**, **Caillat2011**] and its spectrally-resolved variant, the Rainbow RABBIT [**Gruson2016**].

In the present study, we combined Rainbow RABBIT attosecond spectral interferometry with VMI momentum spectroscopy to record the modulus and phase variations of the photoelectron quantum state with high spectral resolution and angular sensitivity. This was performed in the test case of two-photon XUV+IR photoionization of helium through the intermediate resonant states $1s3p$ and $1s4p$. The resulting structured photoelectron wavepacket was fully characterized by measuring quasi-continuously (over a 800-meV range) the spectral and spatial variations of the two-photon transition amplitude $M(E,\theta)$. The latter display rich structures such as sudden phase jumps of up to π rad *in both dimensions* [**Autuori2022**].

These measurements give direct access to the complete, angularly-resolved, dynamics of the two-photon transition leading to photoemission [**Vacher2017**]. The angularly and spectrally resolved ionisation rate, obtained by a Gabor analysis of the experimental $M(E,\theta)$ using a sliding 210-meV Gaussian window, is shown in Fig. 1 for two illustrative angles. *At resonances*, i.e. around $E_{1s3p} + \hbar\omega_0 \approx 0.06$ eV and $E_{1s4p} + \hbar\omega_0 \approx 0.66$ eV (indicated by blue and red dashed lines resp.), the dynamics is globally delayed due to the transient trapping of the electron in the intermediate bound states before completing the transition. *Between resonances*, the dynamics is strongly shaped by quantum destructive interferences, appearing as 'holes' in the spectro-temporal maps. These 'holes' shift towards higher energies when θ increases, e.g., from 0.33 eV at 0° to 0.59 eV at 65°, illustrating the high spectral *and* angular dependences of the photoemission dynamics.

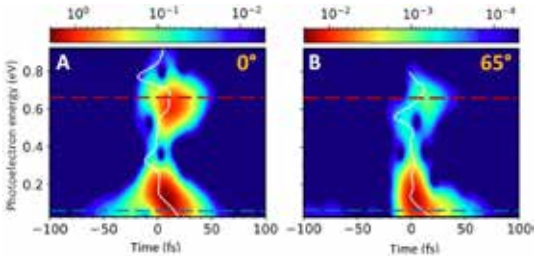

Figure 1. Spectrally and angularly resolved ionisation rate obtained by a Gabor analysis of the two-photon transition amplitude $M(E,\theta)$ at $\theta = 0°$(A) and $\theta = 65°$(B). The transition delay defined as the *local* spectral derivative of $\arg M(E,\theta)$ is overlaid as white lines on each Gabor representation.

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Rabi Dynamics Driven by a Seeded FEL at XUV-wavelengths

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Sinusoidal population transfers in two-level quantum systems, due to resonant external fields, are known as Rabi oscillations. While long-wavelength Rabi oscillations are frequently used in cavity quantum electrodynamics, short-wavelength Rabi oscillations have so far not been observed experimentally. In this work [1], we demonstrate that it is possible to drive Rabi oscillations at extreme-ultraviolet (XUV) wavelengths using intense pulses from a seeded free-electron laser (FEL) [2]. Our experiments are performed on helium atoms between two states: $|a\rangle = 1s^2\,(^1S_0)$ and $|b\rangle = 1s4p(^1P_1)$ with an atomic resonance at $\hbar\omega_{ba} = 23.742\,\text{eV}$.

Ultra-short FEL pulses of $56 \pm 13\,\text{fs}$ duration are shown to trigger Rabi oscillations with a period of $2\pi/\Omega \approx 52\,\text{fs}$, which implies ultra-fast Rabi dynamics in the single-cycle regime. Measurements are performed in-situ by recording electrons from two-photon ionization processes of the helium atoms. The photoelectron signal splits up into a doublet structure, identified as an Autler-Townes (AT) doublet [3], when the FEL frequency is blue detuned relative to the atomic resonance by $\Delta \approx 11\,\text{meV}$.

While the AT splitting was expected [4], we find that it exhibits a strong asymmetry with detuning of the FEL frequency that can not be explained as a breakdown of the rotating wave approximation, due to the weak-coupling condition: $\omega \approx \omega_{ba}$ and $\Omega/\omega_{ba} = 0.34\%$ [3]. Instead, the recorded asymmetry shows that the high intensities of the FEL pulses balance photoionization rates of one-photon ionization from the excited state: $|b\rangle$, with non-resonant two-photon ionization from the ground state: $|a\rangle$. This results in a complex interference phenomenon that explains the blue shift of the observed AT doublet.

Our experimental observations are supported by ab initio simulations based on the time-dependent configuration-interaction singles (TDCIS) method [5]. Furthermore, we have developed an analytical model, based on a Dyson series of the Rabi oscillating two states, that quantitatively explains the interference and decay mechanisms of Rabi oscillations at short-wavelengths [1].

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Wave-packet dynamic in a SU(2) non-Abelian Gauge field

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Non-Abelian gauge field plays an important role in high-energy physics for example in Yang-Mill theory, in condensed-matter physics, for instance, with anomalous quantum Hall effect, and in quantum information. In its SU(2) symmetry version, Hamiltonians with non-Abelian gauge field might reduce to spin-orbit coupling-like systems, taking the form: $H = \boldsymbol{p}^2/2m + \boldsymbol{A}.\boldsymbol{p}/m$, where m is the mass of the particle, $\boldsymbol{p}$ the momentum and $\boldsymbol{A}$ the non-Abelian gauge field with *2x2* matrix components, decomposed on SU(2) Lie group generators. These class of Hamiltonians can be simulate with ultracold gas [1] using various methods [2]. The topological properties of spin-orbit-coupled system have been explore analysing the energy bands in 2D Fermionic system [3]. Here, the eigenenergies have momentum dependence, leading to Rabi flopping with periodic change of quasi-momentum, even if the non-Abelian gauge field is homogenous. This oscillation is similar to relativistic Zitterbewegung predicted in Dirac equation and simulated in ultracold system [4].

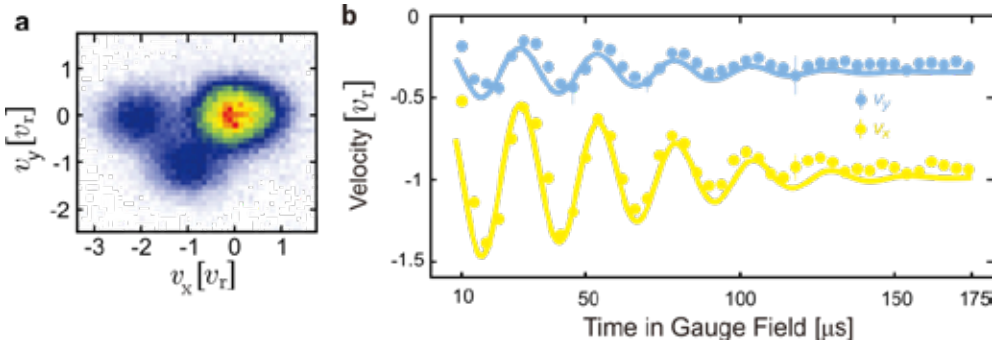

FIG. 1: **a** Time of flight of the gas after interaction with the gauge field. **b** Oscillation of the wave-packet of velocity component, for a momentum amplitude of $p = 5.6p_r$ (p_r: recoil momentum).

We present recent experiments of the dynamic of an atomic wave packet in a bi-dimensional synthetic non-Abelian gauge field using an ultracold Fermionic gas. In Fig. 1a we show a typical three peaks velocity distribution and in Fig. 1b we show an example of wave-packet velocity oscillation. The damping oscillation is due to the finite temperature (Here, $T = 45$ nK) of the gas. Exploring the evolution of the oscillation in the plane of the non-Abelian gauge, we found that the oscillation is normal to the wave packet momentum indicating that the dynamic is due to spin Hall effect. Moreover, the oscillation amplitude is anisotropic with complete suppression of the oscillation for specific momentum orientation [5]. We will give a clear physical interpretation of this phenomenon and discuss application of non-Abelian gauge field in quantum information [6] and atomtronics [7].

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Quantum fluids of light in hot atomic vapors

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Hot atomic vapors are widely used in non-linear and quantum optics due to their large Kerr non-linearity. This non-linearity induces effective photon-photon interactions allowing light to behave as a fluid displaying quantum properties such as superfluidity [1].
Quantum fluids of light rely on the analogy between the non-linear Schrödinger equation (NLSE) describing the propagation of light in non-linear media and the Gross-Pitaevskii equation (GPE) describing a weakly interacting Bose gas :

$$i\hbar\frac{\partial}{\partial t}\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V + g|\psi|^2\right)\psi \quad \textbf{\textit{(GPE)}}$$

$$i\frac{\partial}{\partial z}E = \Big(\underbrace{-\frac{1}{2k_0}\nabla_\perp^2}_{\textbf{Kinetic}} \underbrace{-\,\delta n(\mathbf{r})\frac{k_0}{2}}_{\textbf{Potential}} + i\frac{\alpha}{2} \underbrace{-\,n_2 k_0|E|^2}_{\textbf{Interaction}}\Big)E \quad \textbf{\textit{(NLSE)}}$$

In this presentation we will show that we have full control over the three terms and we can engineer an analogue simulator with light. We control the initial kinetic energy distribution by sending intensity fluctuations on top of a gaussian background fluid, and measure the coherence of these fluctuations. We observe the emergence of a prethermal state [2] with long range order, with a topological phase transition precursor. With increasing fluctuation intensity, the coherence function switches from an algebraic to an exponential decay, strongly reminiscent of a BKT transition.

By studying the effect of interaction quenches in the fluid [3], we evidence the dynamical Casimir effect i.e the spontaneous emission of correlated pairs of phonons. Employing Bragg spectroscopy, we measure the static structure factor of our fluid of light [4], confirming the similarity between our photon-photon interactions and interatomic interactions in a BEC.

Finally, we merge novel characterization tools [5] and all optical potential in our latest experimental setup. Using beam shaping techniques, we realize arbitrary potential shapes and sign, allowing to explore new effects arising from confinement.

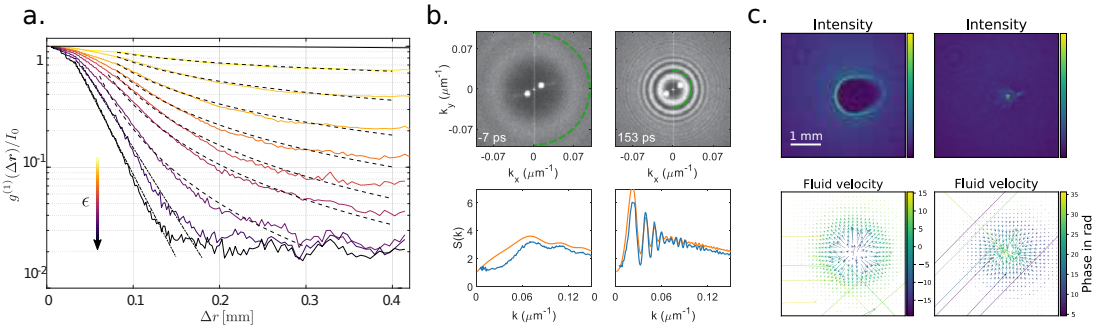

Figure 1: a. First order correlation function with increasing fluctuation strength ϵ, transition from an algebraic to an exponential order. b. Quench induced correlations in the structure factor of the fluid for different evolution times after the quenches. c. Scattering of the fluid on an attractive or repulsive defect.

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Manifestation of relative phases in collision of Bose-Bose droplets

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We study collision of two Bose-Bose droplets [1]. We take into account the initial phase difference between the wavefunctions describing the two components of left and right droplet. A variety of different scenarios of collision is predicted. Description of the process, based on the two coupled Gross-Pitaevskii equations is compared to a simplified model which accounts for the zero-modes only. This model allows to interpret the collisions in terms of a two-component dynamical Josephson junction.

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Precision Measurements and Pauli Blocking with Quantum Degenerate Metastable ^{3}He

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Precision measurements on calculable systems are commonly used for tests of highly involved quantum electrodynamics (QED) calculations and are sensitive probes for the discovery of new and unexplored areas of physics. In our experiment we apply laser cooling and trapping techniques on helium atoms, to perform a highly accurate measurement on the doubly forbidden $2^3S_1 \rightarrow 2^1S_0$ transition at 1557 nm. This serves as a test of QED calculations and as a means to extract information on nuclear charge radii from the ^{3}He - ^{4}He isotope shift of this transition, in view of the recent developments around the so-called 'proton-size puzzle'.

Our most recent experiment involves the measurement of this transition at a targeted 10^{-12} accuracy in a degenerate Fermi Gas of ^{3}He, confined in a dipole trap at the 319.8 nm magic wavelength. In this configuration, the spectral lineshape is purely dominated by the Fermi-Dirac statistics of the gas, and showcases a remarkable sub-Doppler narrowing effect due to Pauli blockade of stimulated emission in the dense part of the cloud. Our modeling and tests of this unexpected effect confirm the first observation of Pauli blockade in a coherently driven system. [**1**]

The targeted accuracy of the ^{3}He transition itself sets a solid benchmark for electronic structure calculations, as does a precise evaluation of the magic wavelength condition. When combined with our earlier result on bosonic ^{4}He [**2**] to obtain the isotope shift, the measurement will provide the most accurate determination of the nuclear charge radius difference between the alpha and helion particle.

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Non-equilibrium state preparation in driven-dissipative atomic quantum gases

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A system of ultracold atoms can be brought in contact with a thermal bath by letting it interact weakly with a large cloud of another atomic species. We consider atoms in a time-periodically driven optical lattice in contact with an interacting Bose condensate and microscopically model them using Floquet-Born-Markov theory. The interplay of driving and dissipation will guide these systems into non-equilibrium steady states. Compared to the usual adiabatic state preparation, suffering from non-adiabatic excitation processes, this scenario can have two advantages; it is robust, since energy (and entropy) can be dumped into the bath, and it allows for the preparation of interesting states beyond the strict constraints of thermal equilibrium. I will present two examples in rather different regimes: (i) In a system of fermions loaded into the Floquet-topological band structure of a hexagonal lattice created by high-frequency driving, the coupling to the environment allows to "cool" almost all particles into a single band so that a topological insulator giving rise to a quantized Hall response is prepared [1]. (ii) Subjecting a one-dimensional bosonic system to a spatially local drive of intermediate frequency that resonantly excites (heats) the system, the interplay of driving and dissipation is found to give rise to the formation of a non-equilibrium Bose condensate in a subspace that approximately decouples from the drive [2]. Finally, I might also mention the (experimental and numerical) observation of a dynamical phase transition occurring at a critical time during the bath-induced relaxation dynamics of an open system [3].

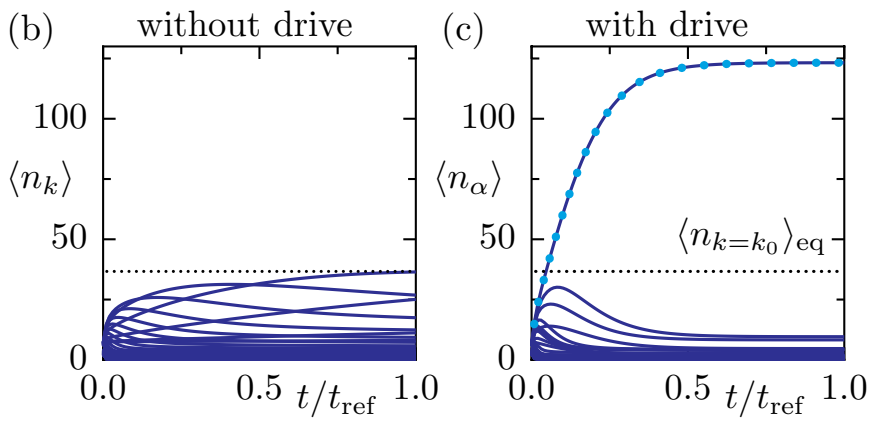

FIG. 1: Time evolution of occupation numbers of an open system with and without drive. The interplay between Floquet heating induced by the drive and bath-induced dissipation causes non-equilibrium Bose condensation in a subspace that decouples from the drive.

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Synthetic Gauge Fields with Ultracold Atoms

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Topological phases of matter exhibit remarkable electronic properties. A prominent example is the robust quantization of the Hall conductivity in quantum Hall insulators. A widespread technique for generating topological band structures in synthetic quantum systems, such as ultracold atoms in optical lattices, is Floquet engineering. This method relies on the periodic modulation of the system's parameters to emulate the properties of a non-trivial static system. The rich properties of Floquet systems, however, transcend those of their static counterparts. The associated quasienergy spectrum can exhibit a non-trivial winding number, which leads to the appearance of anomalous chiral edge modes even in situations where the bulk bands have zero Chern numbers. Here, I report on the realization of such an anomalous Floquet topological system in a periodically-modulated hexagonal optical lattice and show how wavepacket dynamics can be used to study the bulk [1] and edge topological properties of the system. The novel properties of topological Floquet phases open the door to exciting new many-body topological phases without any static analog.

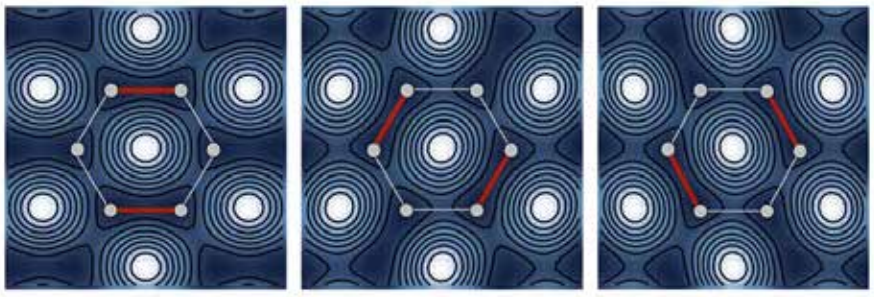

FIG. 1: Three instances of time of a periodically-modulated honeycomb lattice. The gray circles mark the lattice sites and the solid lines indicate nearest-neighbor tunneling within the unit cell. The red solid lines show increased tunneling along a specific bond, which is modulated as a function of time.

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Probing of the ground-state atomic alignment-to-orientation conversion in an external magnetic field with different polarizations of the probe beam

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In the present work we show results from an investigation of atomic angular momentum alignment-to-orientation conversion (AOC) by observing absorption signals of cesium atoms. The AOC is created by combined action of linearly polarized D1 pump laser radiation and an external magnetic field. Due to the nonlinear dependencies of the energies of ground-state and excited-state magnetic sublevels, the transverse angular momentum alignment, created by the exciting linearly polarized light, can be partially converted to orientation. Then the system is probed by a weak circularly polarized D2 laser, as circularity is direct evidence of angular momentum orientation. The excitation and observation geometry for creating and observing AOC stands as follows: the magnetic field **B** defines the quantization axis, and the exciting linearly polarized laser radiation **E** forms an angle of $\pi/4$ with respect to the magnetic field **B**, the probing direction is in the direction perpendicular to both **E** and **B**.

The theoretical model is based on the optical Bloch equations and uses the density matrix formalism. The theoretical model takes into account all transitions, the mixing of magnetic sublevels in an external magnetic field, the coherence properties of the exciting laser radiation, and also includes averaging over the Doppler profile [1]. In the present work we analyze the influence of the probe laser polarization on the absorption signals, in particular, on the difference signals between two counter circularly polarized absorption components. We have modeled the signals for various probe beam polarization states: from linearly polarized to elliptically polarized with different phase and azimuth angle values.

Our results show that for the ideal azimuth angle of the probe beam polarization, which is $\pi/4$ with respect to the magnetic field **B**, the phase values do not impact the signal much, however when the azimuth angle deviates from the ideal case the absorption signals become contaminated with the linearly polarized difference signal becoming the dominant part in the difference signal shape, as it is several orders of magnitude larger than the angular momentum orientation contribution to the signal.

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Dual Comb Spectroscopy for Electronic Fingerprinting

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Dual Comb Spectroscopy combines high spectral resolution with broad spectral coverage and short measurement times. In the recent years, this spectroscopic method has proven its capabilities in molecular spectroscopy in different spectral regions ranging from the visible across the infrared spectral region into the THz domain [1-3]. The UV has so far been neglected for fingerprinting although electron transitions are as element specific as rovibrational transitions and the corresponding absorption cross sections can be huge (> 100 Mb). Especially molecular gasses of astrophysical and environmental relevance have strong and congested absorption characteristics in this spectral region (few examples: NO_2, CO, SO_2, HCHO). I will present our latest efforts on expanding dual comb spectroscopy via nonlinear frequency up-conversion into the ultraviolet region. The challenges include UV frequency comb generation with a high photon flux, efficient UV interferometry and fast UV signal detection [4].

Figure 1 shows the principle of ultraviolet dual comb spectroscopy (UV-DCS) and a state of the art NUV absorption spectrum of HCHO recorded with a traditional scanning technique yielding a relative spectral resolution of 10^{-6}. This resolution has not been sufficient to determine the absolute absorption cross section of formaldehyde so far [5]. UV-DCS has the potential to eliminate this shortcoming by improving the relative spectral resolution by one order of magnitude in single shot measurements. By further improving the long-term performance, an ultra-high relative resolution of up to 10^{-10} and an unrivaled simultaneous spectral coverage on the order of 100 THz comes within reach.

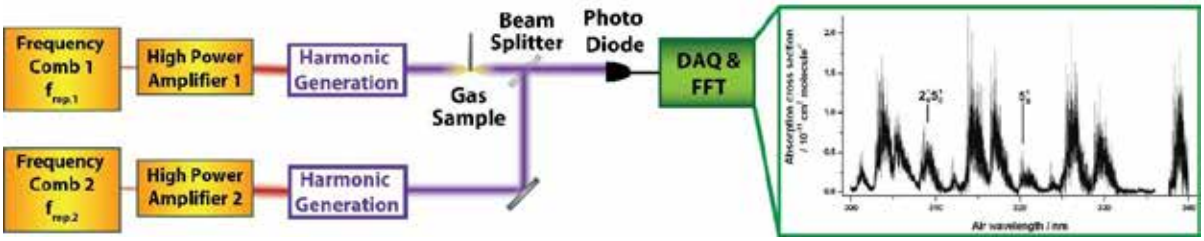

Figure 1: Setup for ultraviolet dual comb spectroscopy. The outputs of two amplified frequency combs with slightly different repetition rates are frequency-up-converted into the ultraviolet spectral range were many molecular and atomic samples exhibit strong and congested absorption features. After one comb interacted with the sample, the two beams are superimposed and the interference is detected with a photo diode. The Fourier transformation of the time-domain interferogram reveals the absorption spectrum of the sample (DAQ & FFT). Example: state-of-the-art NUV spectrum of HCHO whose spectral resolution has not been sufficient for determining the absolute absorption cross section [3]. UV-DCS promises at least a 10-fold improved spectral resolution in single shot operation.

Acknowledgements

This project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (grant agreement no. 947288) and from the Austrian Science Fund FWF START programm (grant agreement no. Y1254N).

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Cavity mode-dispersion spectroscopy

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Mode pushing is a well-known linear phenomenon that occurs in an optical cavity with an absorbing medium. However, exceptionally accurate and precise measurements of molecular spectra that are derived from measurements of such mode frequency shifts have only recently been demonstrated. The success of this technique can be ascribed to the intrinsic physical connection between absorption and dispersion as well as by enabling technical advances in experimental techniques including tight laser frequency locking to high-finesse cavities via the Pound-Drever-Hall method, laser frequency control with sub-Hz-level accuracy, high-bandwidth heterodyne detection of optical signals, and the use of clock-referenced optical frequency combs.

For experiments that involve high-finesse optical cavities containing an absorbing gas, measurements of mode frequencies with uncertainties at the sub-Hz level provide all the information from which the dispersion spectrum of the sample can be accurately constructed. This technique is referred to as cavity mode-dispersion spectroscopy (CMDS), with its primary observable being frequency [1]. Because of the frequency-centric nature of the measurement, CMDS is immune to bias caused by nonlinearity in the detection of light intensity and which adversely affects most other spectroscopic approaches. Recent examples of CMDS-based measurements that were traceable to primary frequency standards of the SI include, molecular transition intensities determined with sub-promille relative uncertainty [2], Doppler-free saturation spectroscopy of weak molecular transitions yielding results demonstrated to be superior to other techniques [3], a broadband experiment involving an optical frequency comb and a Fourier transform spectrometer [4] and finally a fast dual-comb detection scheme [5,6]. Using frequency-locking methods and heterodyne detection, one can now precisely measure the time-dependent interference between the transient cavity field oscillating at the mode frequency and that of a local oscillator which is precisely detuned from this resonance. In this fashion one can rapidly measure the mode frequency on a time scale that is much shorter than the cavity decay time. This result was demonstrated using the cavity buildup dispersion spectroscopy (CBDS) technique, [7] and subsequently in a broadband experiment using dual-comb cavity ring-down spectroscopy (DC-CRDS) [8].

These developments make pure frequency-based dispersive spectroscopy an attractive alternative to conventional approaches based on intensity-based measurements of cavity decay rates or light absorption - especially in studies of weak molecular transitions. Applications include reference data for a new generation of spectroscopic databases, measurements of fundamental physical constants, experimental validation of theories of

molecular spectra, research on global warming and exploration of exoplanets, and the search for new physics beyond the Standard Model in molecular systems.

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A Decade with Quantum Biology: How Non-Trivial is Quantum Mechanics of Photosynthetic Light-Harvesting?

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In 2007, Nature published an article reporting evidence for wavelike energy transfer in the Fenna-Mattews-Olson complex, a small photosynthetic antenna isolated from green bacteria [1]. This publication marks a start of an attempt by physicists to revolutionize biology and open its door to quantum mechanics. Much interest has initially revolved around the distinction between trivial and non-trivial quantum effects. In this contribution, we will briefly describe the past decade and a half of development in the theoretical understanding of excitation energy transfer in photosynthesis under the new quantum paradigm in this field. While the field has shown steady progress, directly related to the finds of [1], we demonstrate that concepts ill-defined in the context of photosynthesis research and imported from other branches of physics actually hindered understanding of important natural photo-physical processes. In particular, the classification into the classical, quantum, and non-trivially quantum behaviors has been based on an incorrect understanding of the classical limit of photosynthetic energy transfer [2, 3, 4]. In the emerging field of quantum biology, many hopes were placed on the difference between the supposed true quantum behavior of individual molecules and the inherently averaged behavior of the spectroscopically observed molecular ensemble in which quantum effects get washed out. At least some of the crucial proposals of quantum biology were motivated by the idea that the basic tool of open quantum systems theory, the reduced density matrix (RDM), only represents a statistical average over a molecular ensemble and that something more profound can be found by circumventing the average. We will argue that while the reduced density matrix (adequately applied) always leads to the correct computational results, it indeed blurs the picture of an open system's state, especially in relation to the state of its environment. The density matrix formalism, for instance, does not distinguish between decoherence and dephasing and thus makes it difficult to discuss entanglement between the open system and its bath. Thus the intuition that RDM represents a conceptual problem can be confirmed as correct. However, in the early quantum biological efforts, the uncertainty in interpreting coherence-related processes by RDM paved the way for the "classicalizing" interpretations of microscopic processes of interaction between molecular systems, their environment, and light. Most such interpretations were based on the traditional but loosely reflected Copenhagen interpretation of quantum mechanics with its imposition of preexisting classical concepts and states [4]. We propose that conceptual problems in molecular physics require their own interpretational framework, which sees classical states as emerging from quantum theory. State vector picture of open quantum systems is the most suitable conceptual tool to become a basis for such a framework. We provide several examples of conceptual questions from quantum biology and beyond, which can be decided (only) from the state vector point of view. We will demonstrate that quantum entanglement is crucial for photosynthetic antennae's function, albeit in a radically different context than initially proposed in quantum biology. We argue that the combined use of the density matrix and state vector representations as computational and conceptual tools, respectively, brings a serious advantage over the density matrix alone.

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Reversing time with ultra-cold atoms for quantum *undo* operations.

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We report on an entropy rectification method that makes use of optimal control strategies to faithfully time-invert the dynamical evolution of a Bose-Einstein condensate (BEC) of ^{87}Rb atoms realized with an atom-chip for *undo* operations in quantum regimes. Our work explores several time-reversal experiments by letting the BEC evolve through different paths in the five-fold Hilbert space given by the $F = 2$ rubidium hyperfine ground state (Fig. 1). The optimal backward evolution is achieved by using gradually higher level of control in terms of the complexity of the addressed control problems. Specifically the time-inversion is realized by means of a radio-frequency pulse modulation designed with a dressed Chopped Random Basis (dCRAB) algorithm [1,2]. The experimental results show how this technique successfully works in bringing the system back to its initial conditions with an average accuracy of 92%. Our findings can be applied for the practical realization of quantum *undo* operations which in some platforms, like the gate-based one presented in this work, can be related to the time-reversal of the last performed operation. We believe that the experiments we realized constitute the proof-of-principle of a wide class of quantum *undo* operations to be implemented in several quantum technologies contexts.

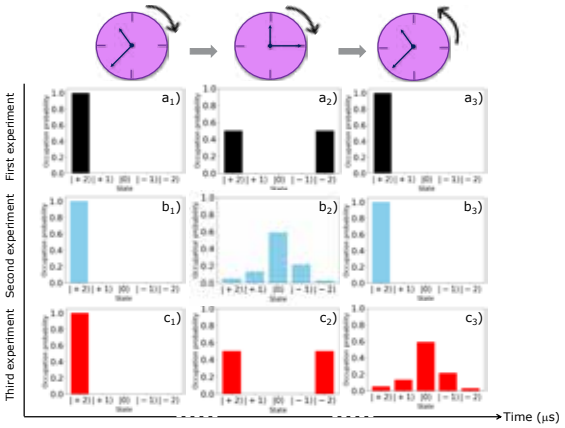

Figure 1: Pictorial representation of the realized time-reversal experiments.

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“Towards attosecond imaging at the nanoscale using extreme ultraviolet high harmonic sources”.

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Ultrafast lasers enable the generation of extremely short attosecond pulses in the extreme ultraviolet region via high harmonic generation. While the ultrashort pulse duration enabled groundbreaking spectroscopic studies of ultrafast electron dynamics on their fundamental attosecond time scales [1], the short wavelength and the excellent spatial coherence enables imaging with nanoscale spatial resolution [2].

In my talk, I will present our recent achievements in the latter field, namely achieving 16 nm spatial resolution, quantitative amplitude and phase contrast as well as chemical mapping of a semiconductor device on the nanoscale. These results have been enabled by combining a highly- stable, high photon-flux, table-top EUV source with an interferometrically stabilized ptychography setup, structured EUV illumination and advanced phase-retrieval algorithms [3].

In a second part I will discuss the challenges of combining high spatial and temporal resolution in ultrafast pump-probe imaging experiments and present a novel approach to deal with the large spectral bandwidth of attosecond pulses, which usually hinders high resolution coherent diffraction imaging [4]. I will present our novel broadband diffractive imaging scheme, which combines multiple-reference wave holography, directional Fourier-filters and a broadband phase retrieval algorithm to retrieve a monochromatic high resolution image.

In a proof of principle experiment, we demonstrate a spatial resolution of 34 nm (2.5 times the illumination wavelength of 13.5 nm) in combination with a spectral bandwidth supporting a Fourier limited pulse duration of only 380 as. The method is single-shot capable, additionally retrieves the spectrum from the measured diffraction pattern, and is thus immune against shot-to-shot fluctuations. This paves the way for an ultrafast view on nanoscale dynamics e.g. ultrafast charge transfer or ultrafast spin currents being relevant for Petahertz electronics and future data storage.

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Influence of Shape Resonances on the Angular Dependence of Molecular Photoionization Delays

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Ultrafast photoionization dynamics in molecules has recently drawn much interest with extreme ultraviolet (XUV) attosecond light sources becoming available and pioneering (XUV-IR) pump-probe experiments on atomic, molecular and solid targets were conducted to characterize photoionization time delays. In molecules, one-photon ionization delays are challenging to retrieve in such experiments because of congested electron energy spectra and the non-spherical symmetry of molecules. The latter causes an intrinsic anisotropy of the molecular potential, which was predicted to lead to a rich angular dependence of the one-photon ionization time delay in the molecular frame for diatomics [1]. The one-photon ionization time delay is defined as the energy derivative of the phase of the complex-valued photoionization dipole amplitude (PDA), which is experimentally accessible through measuring the molecular frame photoelectron angular distribution (MFPAD), i. e., the emission probability relative to the molecular axis, and extracting the constituting partial wave dipole matrix elements.

In this work, photoionization time delays were completely resolved in the molecular frame for inner-valence ionization of NO($X^2\Pi$) into the $NO^+(c^3\Pi\ 4\sigma^{-1})$ state by measuring the MFPADs at the PLEIADES and DESIRS beamlines of synchrotron SOLEIL at a fine energy spacing between 23.25 and 38.75 eV photon energy across the $4\sigma \rightarrow k\sigma^*$ shape resonance. FIG. 1 shows the evolution of the MFPAD for an orientation parallel to the polarization which undergoes dramatic changes as a function of the photon energy and the pronounced molecular frame angular dependence of the ionization delays. A multichannel Fano model reveals that the observed angular dependence of the time delay is well predicted considering the coherent superposition of an angle-independent resonant component and an angle-dependent non-resonant component [2]. The angle-resolved one-photon ionization delays for NO obtained in this spectrally resolved synchrotron experiment will be interesting to compare with recent results based on attosecond XUV+IR pump-probe experiments [3]. The methodology to determine photoionization delays from synchrotron measurements is also applicable to inner-shell ionization as shown independently in parallel for core ionization of CO molecules [4].

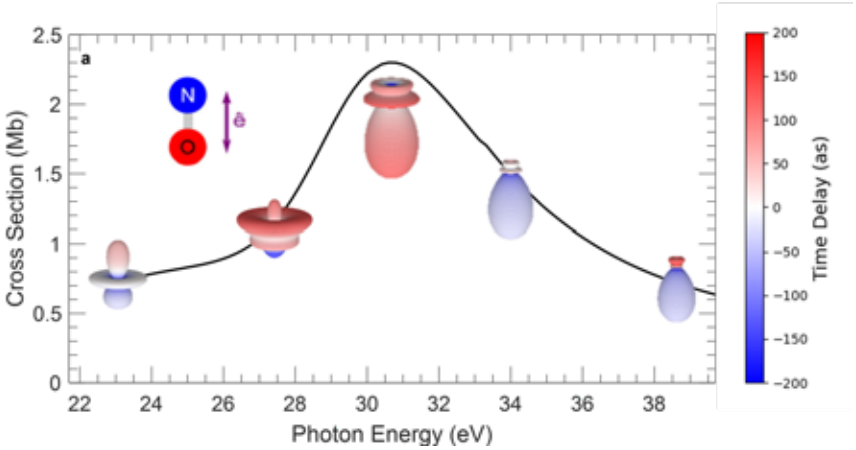

FIG. 1: Photoionization cross section and evolution of the MFPAD and photoionization time delay for inner-valence ionization of NO as a function of the photon energy.

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Tightly-Focused Elliptically Polarized Light: a Highly Efficient Tool for Chiral Discrimination

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Distinguishing between the two opposite versions (enantiomers) of a chiral molecule is vital in organic chemistry, materials science or biomedicine, but also challenging, as they behave identically unless they interact with another chiral object. Standard chiral light, i.e. circularly or elliptically polarized light, is a convenient chiro-optical tool [1], but it is highly inefficient: the enantio-sensitive response of the molecules arises beyond the electric-dipole approximation and is only a small fraction of the total optical response.

Here we show that that tight focusing can turn an ultrashort elliptically polarized pulse into a highly efficient chiro-optical tool. The longitudinal components that naturally arise upon tight focusing [2] leads to enantio-sensitive *bending* of the nonlinear optical response. The reason is that when an elliptically polarized laser is tightly focused, the laser polarization plane tilts towards the propagation direction, as depicted in Fig. 1a. This tilt is opposite at opposite sides of the beam axis and is locked to the propagation direction. In an ultrashort laser pulse, the combination of the tilted electric-field vector with the propagation direction creates a chiral structure that allows us to distinguish between opposite enantiomers via purely electric-dipole interactions.

Figs. 1b,c show that the proposed optical configuration leads to enantio-sensitive bending [3] of the non-linear optical response of randomly oriented chiral molecules: opposite molecular enantiomers emit harmonic light in opposite directions, and thus the enantio-sensitive direction of bending records the molecular handedness with high efficiency. Interestingly, this strongly enantio-sensitive effect is driven by purely electric-dipole interactions, even though the optical field is not locally chiral, making this optical driving field fundamentally different from our previous proposals [3,4] and, to our knowledge, from any other optical setup for chiral recognition, thus creating new opportunities for ultrafast and efficient imaging of molecular chirality and attosecond chiral dynamics.

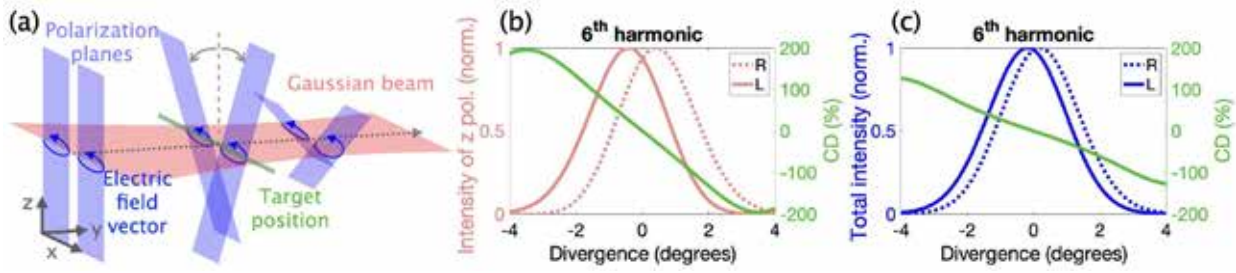

FIG. 1. (a) Forward polarization tilt (blue) in an elliptically polarized gaussian beam (pink), tightly focused into a chiral medium (green). (b,c) Intensity of the z-polarized component (b) and total intensity (c) of the 6th harmonic emitted by the right- (dotted lines) and left-handed (solid lines) propylene oxide, and spatially-dependent chiral dichroism (green), CD=2(I_L-I_R)/(I_L+I_R); TDDFT simulations, I=6·10^{13}W·cm^{-2}, focal diameter 5μm, λ=780 nm, and pulse duration 7 fs.

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Observing the complex dynamics in uracil via simulated XUV spectra

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The nucleobase uracil exhibits a high photostability due to its ultrafast relaxation process mediated by a S_1/S_2 conical intersection (CoIn) seam. Here especially the interplay between nuclear and electron dynamics becomes prominent. Applying our NEMol Ansatz[1,2] for coupled electron and nuclear dynamics on the quantum level, we were able to observe a seemingly long-lived electronic coherence for the CoIn-mediated relaxation process in uracil. We will discuss the origin of this longevity and will propose a possible experiment to observe its dynamics. Our method of choice is the time-dependent transient XUV/X-ray absorption spectroscopy, since this method is sensitive to the fast changes in electronic structure. Therefore we calculated the transient XUV spectra for the O, N, and C edges based on the complete wavepacket relaxation dynamics after laser excitation. The calculations were performed at the restricted active space perturbation theory (RASPT2) level of theory as outlined by Rott *et al.*[3].

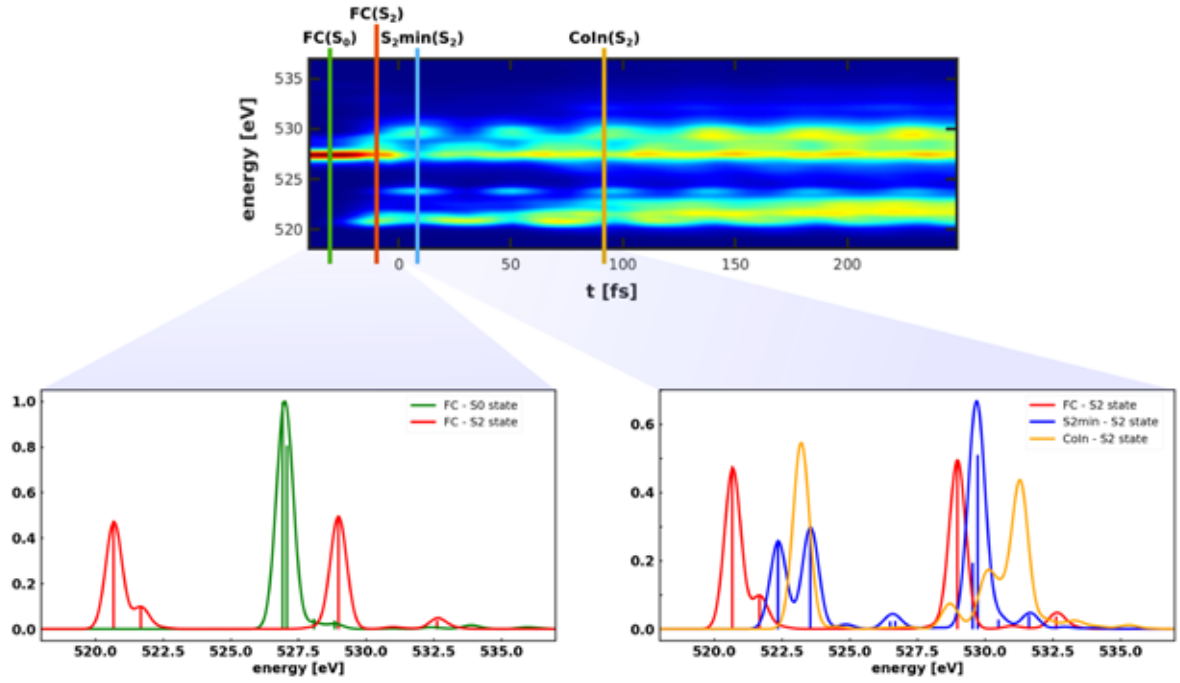

FIG. 1: Time-resolved oxygen K-edge XAS spectrum (top). Static spectra of critical points (bottom) indicated as lines in the top panel. The left side shows the XAS signal at the FC point from the ground state S_0 (green) and the S_2 state (red). The right side shows the XAS signals from the S_2 state at the FC point (red), the S_2 minimum (blue) and the S_1/S_2 conical intersection (gold).

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Sub-cycle Optical Pulses Generated via Parallel Parametric Waveform Synthesis for Attosecond Science

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With the recently experimentally pioneered sub-cycle parallel parametric waveform synthesis [**1**], we access a scalable source for the generation of high-energy optical pulses with full-width-half-maximum (FWHM) pulse durations below one optical cycle (i.e. sub-cycle). We demonstrated the synthesis of down to 0.6 cycle waveforms at 1.4 µm center-wavelength spanning in total from 650 to 2200 nm and with 500 µJ of pulse energy. We characterized the synthesized waveforms via the attosecond streaking technique showcasing their high stability (see Fig. 1a-b). The synthesizer source exhibits the capability to customize the electric field by changing the synthesis parameters between the coherent combination of a near-IR-channel OPA system with another OPA-channel in the IR spectral range. Both broadband OPA-sources have a stable and controllable common CEP, as well as a stabilized relative phase (RP) between the two pulses. These parameters allow for a manifold of sub-cycle waveform customizations. Such waveform control is highly interesting for applications such as high-harmonic generation (HHG) as it enables online-tunable isolated attosecond pulse (IAP) production without the use of additional gating techniques or modification of the HHG-source [**2**]. To date, we demonstrated broadband and tunable HHG between ~30-450 eV in different noble gases. This tunability (see Fig. 1c-e) allows for adaptive IAP generation and can be used in conjunction with a replica of the synthesized waveform for pump-probe experiments. The sub-cycle pulse duration and the tight temporal synchronization to the generated IAP promise to enable strong-field time-resolved experiments with attosecond temporal resolution.

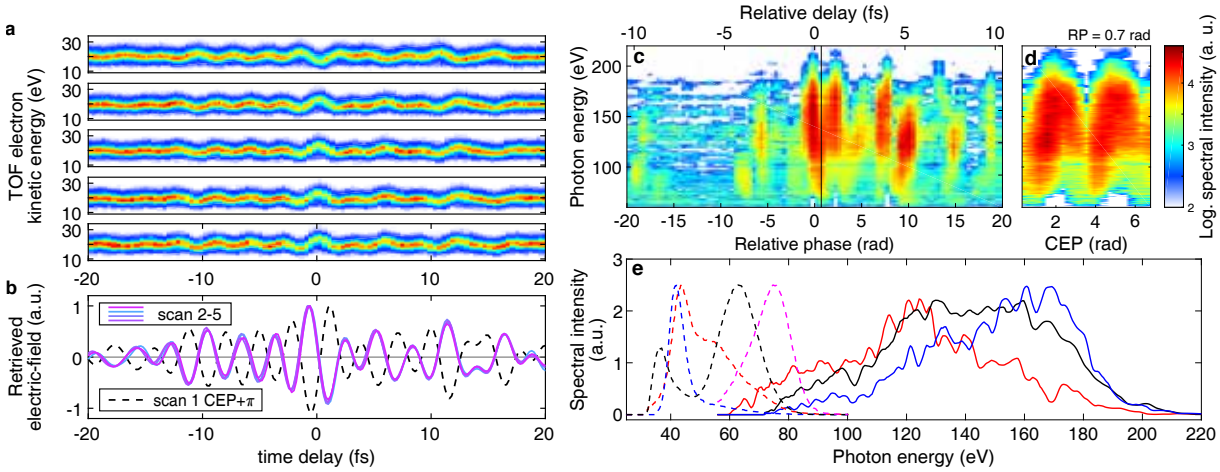

Figure 1: **(a)** Two streaking traces of synthesized sub-cycle pulses with inverted CEP. Three additional traces with the CEP-setting of the 2nd. **(b)** Retrieved electric fields for the five streaking traces above, exhibiting highly repeatable sub-cycle electric field transients. **(c)** Exemplary synthesis scan (here scanning the relative phase) and the corresponding generated high harmonics in neon up to 200 eV. **(d)** CEP-scan at the RP-position marked in c. **(e)** Exemplary tunable HHG-spectra in argon (dashed) and neon (solid).

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A6-1-INV

Studies of reactive and inelastic collisions in a cryogenic multipole trap

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Multipole ion traps have proven to be a versatile tool for precision measurements of reaction rates and spectroscopy [**1**]. Improvements to our 22-pole trap and the development of a new wire trap have resulted in a number of exciting new results from our laboratory.

We present high-sensitivity measurements of the tunneling reaction $D^- + H_2 \rightarrow H^- + HD$, which proceeds via a transient H_2D anion. The measured value agrees with ab-initio quantum tunneling calculations, serving as a benchmark for molecular theory [**2**]. We also present measurements of three-body reaction rate constants of Cl^- with H_2 [**3**]. Furthermore, the addition of a hydrogen atom source allows us to measure the low-temperature reaction rates of atomic hydrogen with carbon-chain anions found in the interstellar medium.

Further work has focused on inelastic collisions of C_2^-, which has been proposed as a candidate for laser cooling due to the existence of multiple stable electronic states. We have demonstrated vibrational state control of C_2^- via a novel scheme that uses optical pumping in conjunction with inelastic collisions of H_2 and measured the vibrational quenching rate [**4**]. Additionally, we precisely determined the proposed laser-cooling transitions of C_2^-. We resolve the spin-rotation splittings and use it to perform accurate thermometry in our newly-developed wire trap [**5**].

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New Insights on The Ozone Formation

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Absorbing UV radiation, ozone (O_3) that exits in the stratosphere protects life on Earth and plays a crucial role in Earth's temperature balance. In contrast, tropospheric ozone is an important greenhouse gas and air pollutant. However, despite its importance and decades of research, the reaction leading to ozone formation is not fully understood due to its complexity. Here, we develop a theoretical approach to model the ozone formation through direct (without invoking the existence of an intermediate complex) ternary recombination reactions O_2+O+M $\rightarrow$ O_3+M where M can be N_2, O_2 or Ar. In particular, we have applied the method to ternary collisions O+O_2+Ar due to the extensive availability of experimental data for comparison. Our formalism is based on classical trajectory calculations in hyperspherical coordinates [1], leading to a fully *ab initio* and pressure-independent rate for ozone formation. Accordingly, thermally-averaged rates were derived for temperatures 5-900K. As a result, it is found that the majority of O_3 molecules formed initially are weakly bound. In addition, accounting for the process of vibrational quenching of the nascent population, a good agreement with available experimental data for temperatures 100-900K is obtained [2].

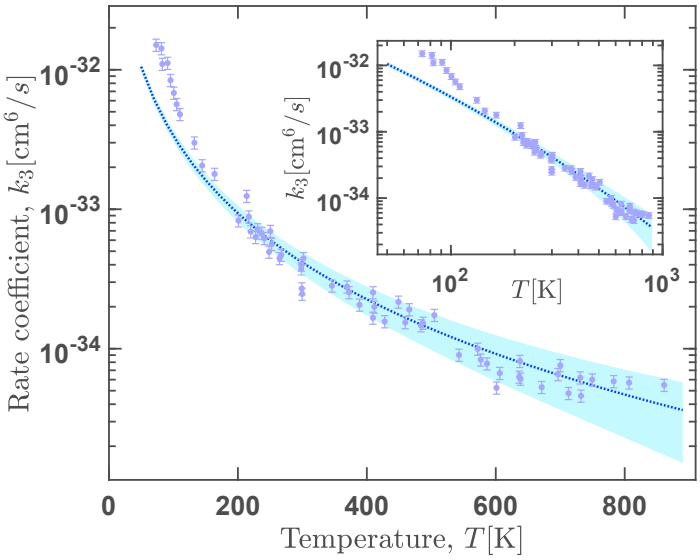

FIG. 1: Thermally-averaged recombination rate coefficients for formation of molecules with all binding energies scaled by the factor of 50 [cm^{-1}]/T accounting for the process of vibrational quenching (solid line). The shaded area (light blue) represents the uncertainty of the theoretical model. The circles with error bars indicate the experimental data.

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A6-3-INV

Title: X-rays from the Universe

Joern Wilms

Most of what we know today about the properties of the hot and energetic universe has been learned using observations with X-rays from satellites. These observations have permitted, e.g., to measure the properties of black holes which accrete material from their surroundings or to determine the state of the plasma in the remnants of supernova explosions or in the gas between galaxies in galaxy clusters. X-ray astronomical measurements rely on the precise knowledge of the properties of inner shell transitions in (often highly ionized) elements heavier than hydrogen or helium. The talk will give an overview of some of the recent results in X-ray astronomy and discuss the data needs for the next generation of X-ray astronomical missions such as the microcalorimeters on the Japanese-American XRISM mission, which is to be launched in 2023.

A Levitating Droplet as a Toy Atom

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There very first example a student learns in a quantum mechanics is the square potential well. However, when working with atoms we use spherical coordinates and a **spherical potential well** would be a much closer analogy. After writing the Schrödinger equation in spherical coordinates, the centrifugal barrier $(\ell(\ell+1)/r^2)$ appears, which, when added to a square potential well in the radial coordinate, results in a wedged potential well.

In this work, we use **an optical trap and a water droplet** to create an experiment with exactly such wedged potential wells. The equation for the scattering intensity obtained directly from the Maxwell equations turns out identical to the radial, Schrödinger equation [1], where the light trapped in resonating modes inside the droplet is analogous to an electron trapped in an atomic potential.

The width of the radial square well is smoothly changed by changing the radius of the droplet resulting in a directional Mie scattering spectrum consisting of a **series of Fano resonances**. This again points to the analogy with an atom, since Fano resonances were first discovered for inelastic electron scattering by helium atoms. The resonances are ordered by the integer angular momentum value, ℓ, associated with the rotation of the light as it reflects inside the surface of the droplet. In an atomic system, this would be the angular momentum of the electron.

The full spectrum consists of a series of consecutive Fano Combs, each with dozens of individual resonances evolving from wide Lorentzian shapes to sharp asymmetrical Fano profiles. We use the analogy with the Schrödinger equation to fully and intuitively explain the Fano Comb structure. This results in a model experiment for an atom with **a knob to control the atom's properties including the potential's width and depth**, that **scans over a wide range of angular momenta**. The spectrum gives a full picture of the range of possible resonances in such a toy atomic system.

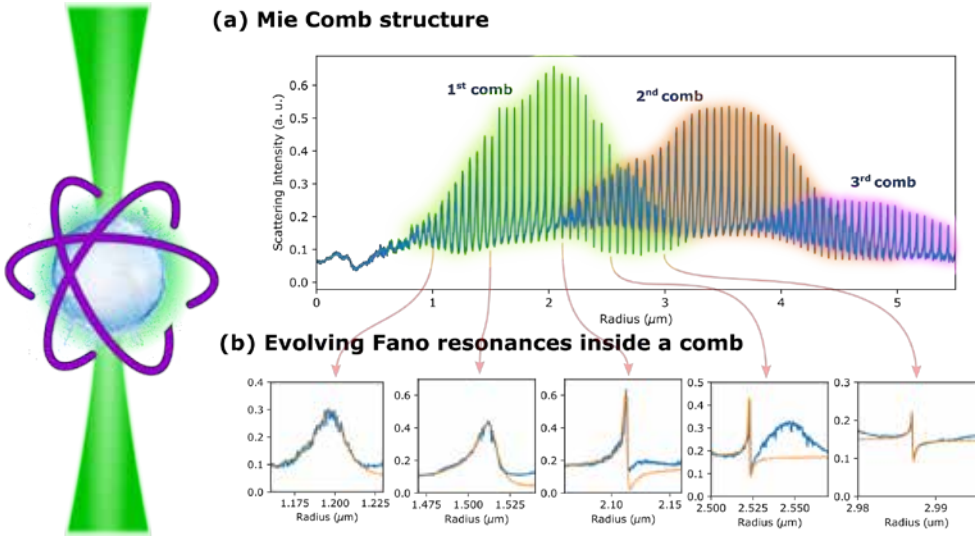

FIG. 1: A water droplet as an atom. **(a)** Scattering intensity of a shrinking water droplet arranged in consecutive *Mie Fano Combs*. Highlighted are the first three *combs* composed of equidistant, evolving Fano resonances. **(b)** Evolution of the resonances from Lorenztians to Fano through five selected segments of the first comb fitted with the Fano equation (orange). These Fano profiles are identical to those observed in photoionization and photodetachment spectra.

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A6-2-HT

Experimental study of X-ray photon-induced desorption from molecular ices: indirect mechanism and astrophysical implications

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The most recent observations of small organic species in the gas phase of the coldest regions of space imply the existence of efficient non-thermal desorption phenomena, central to maintain a sufficient budget of molecules in the gas which should otherwise be depleted by freezing out on interstellar dust grains. This last decade, laboratory experiments have mainly focused on the desorption induced by vacuum UV photons, cosmic rays and recombinative chemistry. However, processes induced by photons of higher energy, despite being present in star and planet formation regions, were largely unknown and neglected in models, until recently. Indeed, X-ray induced desorption from molecular ices has received a peculiar attention in the past few years[4,5,6]. This process, also known as X-ray photodesorption, should participate to the physical and chemical evolution of different astrophysical environments where the X-ray field is important, such as protoplanetary disks, comets and icy moons and planets[7]. Recent investigations[1,2,3] have revealed, in the soft X-ray range, an indirect desorption process that induces the desorption of molecules at photon energy where they are not expected to desorb. This indirect mechanism has major implications and still needs to be fully understood.

In this context, X-ray photodesorption experiments were conducted at the SOLEIL synchrotron facility in France by coupling the Ultrahigh Vacuum SPICES setup to the SEXTANTS beamline, in order to measure desorption yields by mass spectrometry, but also to shed light on the involved mechanisms. Desorption of simple molecules such as ^{13}CO and $^{15}N_2$ was studied as a simple case in order to characterize the indirect desorption process. Resonant 1s core excitation near the N (~400 eV) or O (~500 eV) K-edge, reachable thanks to tunable and high spectral resolution X-rays from the synchrotron beamline, allows to selectively photo-excite $^{15}N_2$ or ^{13}CO to trigger desorption from ices containing these molecules. This first set of experiments allows to discuss the desorption mechanisms and their properties with respect to the energy transport in the ice. Finally, X-ray photodesorption is studied for methanol CH_3OH and other small organic molecules in order to explore the desorption process for more complex molecules, especially relevant for astrochemistry.

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Nonlinear optical phenomena from high repetition rate laser-matter interactions in transparent solids

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Nonlinear propagation of intense ultrashort laser pulses in transparent materials gives rise to a universal phenomenon termed femtosecond filamentation, stemming from a complex interplay between linear and nonlinear effects, which become coupled in space and time through material nonlinearity [1]. This results in nontrivial transformation of pulsed laser beam into a light filament - a very narrow light beam, which develops a complex spatio-temporal structure and carries an ultrabroadband, more than octave-spanning spectrum, termed supercontinuum. Supercontinuum generation in solid state materials at low (kHz) laser repetition rates is well understood and is widely applied in practice as a robust and versatile source of coherent ultracroadband radiation, finding a wealth of applications in modern ultrafast science [2]. However, at high (100s kHz to a few MHz) laser repetition rates, the dynamic picture of femtosecond filamentation in solids becomes considerably altered by accumulation of transient and permanent defects, resulting in gradual modification of the nonlinear material via inscription of self-organized laser-induced periodic surface and volume structures, which share common physical origins [3]. On the other hand, the inscription of self-organized periodic structures gives rise to nonlinear optical side-effects, such as conical third harmonic generation, which readily serves as an early indication of evolving in-bulk optical damage [4,5].

In this Contribution we present the results of conical third harmonic generation that accompanies filamentation and supercontinuum generation in bulk solid-state materials at high repetition rates. It is shown that third harmonic generation obeys noncollinear phase matching condition, which involves reciprocal lattice vector of a nanograting inscribed by femtosecond filament in the volume of transparent material. The existence of a particular nanograting period required to phase match conical third harmonic generation is indirectly verified by investigations of periodicity features of high and low spatial frequency laser-induced periodic surface structures, in which matter is reorganized in a similar fashion. The universality of phenomenon is justified by the observations of conical third harmonic generation in various transparent crystals and glasses and under various experimental settings, such pulse energy, focusing condition and exposure time. These assumptions are further supported by the experiments with tunable femtosecond pulses, producing conical third harmonic emission with ultrabroad spectrum and also revealing the generation of conical fifth and seventh harmonics, which are produced via cascaded four-wave mixing, based on essentially identical phase-matching scenario.

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High-resolution manipulation and imaging of cold atoms through a multimode fiber

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High resolution imaging and tightly focused beams are common tools in cold-atom experiments to image and manipulate atoms. However, with increasing complexity of the setups, the necessary high numerical aperture (NA) of the optical access is a strong constraint on the experimental design. This is particularly true in hybrid experimental approaches that aim at combining cold atoms with other optical, electronic, or opto-mechanical systems. In this context, technologies that allows compact optical access without using macroscopic high NA lenses, are of high interest.

Multimode fibers appear as an elegant solution with 0.5 NA for a transverse size of the order of 100 µm and the ability to flexibly guide light over large distances. The light field at the output of the fiber is linked from its input by a random transformation that creates a speckle profile from a clean Gaussian input beam. However, this transformation is linear and thus it can be inverted. This inversion can be done optically by digital optical phase conjugation with a spatial light modulator (SLM), or it can be performed numerically on the transmission matrix of the multimode fiber after a characterization measurement. Our experimental results show that both methods provide powerful approaches to respectively manipulate and image cold atoms through a multimode fiber.

We use optical phase conjugation to produce almost Gaussian laser beams at the fiber in-vacuum end with a beam injected from the in-air end the wavefront of which we shape with an SLM. First, this allows us to transport rubidium atoms from a magneto-optical trap to 200 µm from the fiber tip. To do so, we implement a moving one-dimensional optical lattice, with one of the two beams formed though the fiber. Second, at the high NA region reached, we demonstrate loading of cold atoms inside optical tweezers shaped through the fiber. The waist of the tweezers can be adjusted down to 1.2 µm and multiple traps with arbitrary geometries can be loaded. Third, we also realize efficient optical molasses to cool the atoms with beams outgoing the multimode fiber [1].

We also demonstrate high resolution imaging through the multimode fiber by numerically inverting the speckle field measured at the in-air side. This imaging requires to first characterize the transmission matrix of the fiber. To do so, we measure by off-axis holography the in-air output field created by a focused beam at the in-vacuum input, the position of the focus being varied with a digital micromirror device in 100×100 µm^2 region. We then perform absorption imaging of cold atoms (see Fig. 1) with resolution of about 1 µm, allowing characterization of the atomic clouds density and temperature in the tweezers [2]. These results pave the way towards the efficient use of multimode fibers in spatially constrained quantum technology platforms relying on cold atoms.

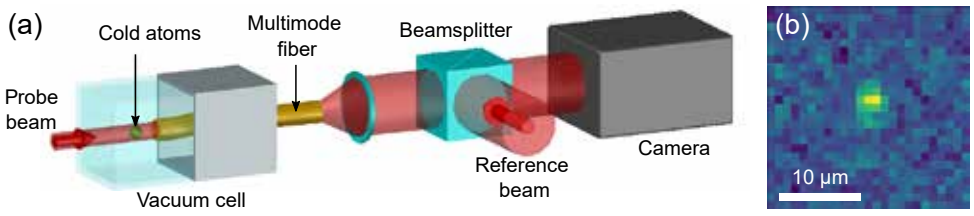

Figure 1: Absorption imaging of cold atoms through a multimode fiber. (a) Setup: the resonant probe beam is transmitted through the fiber and we measure its output speckle field. With the previously characterized transmission matrix of the fiber, we recover the field at the atoms object plane. (b) Image through the fiber of atoms trapped in optical tweezers formed through the fiber.

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Partial cross sections for mutual neutralization involving H^- and D^-

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A key reaction for the ionization balance in various astrophysical environments is the Mutual Neutralization (MN) of atomic or molecular anions and cations: $A^+ + B^- \rightarrow A + B$. Recent studies emphasize on importance of MN in such models [1] and its influence on the determination of stellar metallicities, justifying the large number of calculations recently made for MN involving the hydrogen anion (e.g., [4]). Nonetheless, so far only the reactions involving alkali metal or alkaline-earth cations were compared to experimental data. Those reactions have in common to be limited to Σ molecular symmetries.

We recently upgraded the merged beam setup in Louvain-la-Neuve to reach 5 meV collision energies, and incorporated three-dimensional momentum imaging using two position sensitive detectors located downstream from the region where the A^+ and B^- beams overlap. Besides providing clear coincidence signals between A and B, this technique gives unambiguous identification of LS-terms of the products via the measurement of the kinetic energy release (KER), leading to branching ratios for the $He^+/Li^+/C^+/N^+/O^+ + (H^-)/D^-$ MN reaction for collision energies below 10 meV.

The anion centered asymptotic model (ACAM) [2], was updated in order to take into account non-Σ symmetries. We have found independently that an asymptotic factor should be applied to the anion wavefunction in order to more accurately describe the interaction potential. The remaining discrepancies are explained by atomic configuration mixing.

The partial cross sections produced by ACAM accurately reproduce both the branching ratios measured at UCLouvain and the $Li^+/Na^+/Mg^+ + D^-$ branching ratios [3] measured at DESIREE. The agreement between ACAM predictions and experiments allows us to compute partial cross sections for reactants which are hard to measure experimentally, e.g., $Be^+ + D^-$. The partial cross sections for the $X^+ + H^-/D^-$ will be presented here.

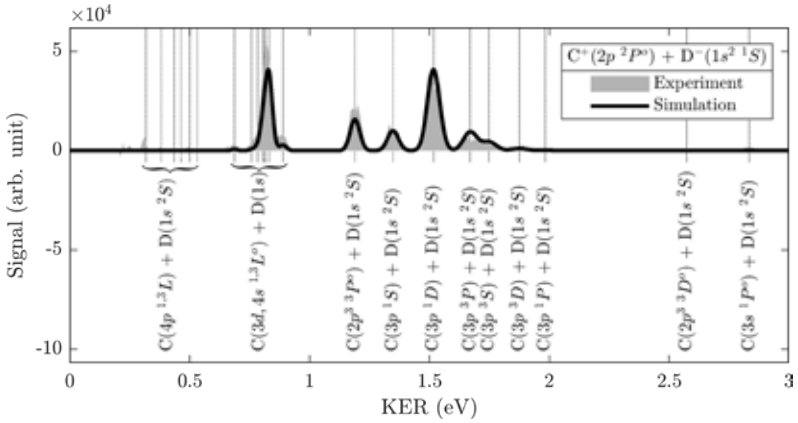

FIG. 1: MN kinetic energy release spectrum for $C^+ + D^-$.

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The Fate of Knockout-Damaged PAHs and Fullerenes: Bridging Ultrashort and Ultralong Timescales

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The advent of cryogenic electrostatic ion beam storage rings and traps has enabled studies of atomic and molecular ions on timescales ranging up to hours. This allows the dynamics of excited species and the transition between different dominating cooling mechanisms to be followed over many orders of magnitude in time. Here, we have studied collisions between polycyclic aromatic hydrocarbon (PAH) or fullerene ions and rare gas targets at velocities close to 100 km/s. At these velocities, which are typical of energetic particles in stellar winds and supernova shockwaves in the regions of space where these molecules are found, one of the dominating destruction processes is the prompt knockout of individual atoms from the molecular lattices on femtosecond timescales [1]. The resulting fragments are highly reactive, far more so than the intact species. Using the DESIREE (the Double ElectroStatic Ion Ring ExpEriment) ion storage rings [2], we have conclusively shown that defect PAH and fullerene ions that have lost a single carbon atom due to knockout cool on millisecond timescales before remaining thermodynamically stable indefinitely in the gas phase [3]. This means that such species are likely to be formed in space and may significantly contribute to the chemical nature of interstellar environments. In my talk I will discuss these results, their potential implications, and how ion storage rings can be used for astrophysical applications.

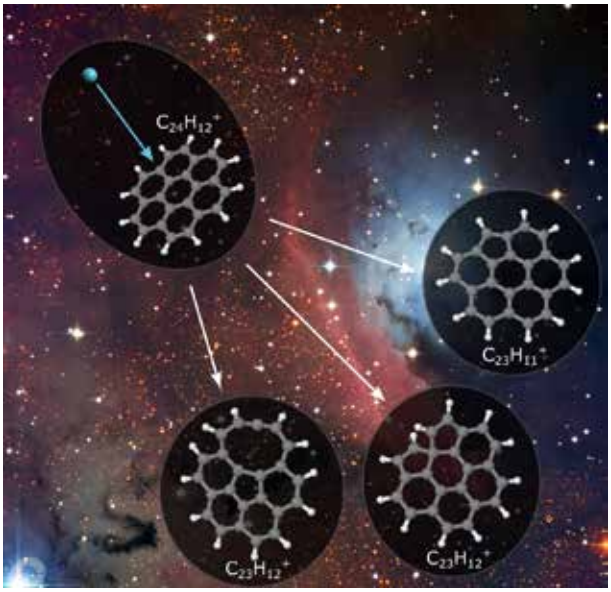

FIG. 1: The knockout of a single carbon atom from a PAH molecule, here a coronene cation ($C_{24}H_{12}^+$), leads to the formation of highly reactive products that are stable on astronomical timescales [3].

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Progress towards a molecular lattice clock to search for time-variation of the proton-to-electron mass ratio

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The search for time-variation of fundamental constant is a promising way to probe physics beyond the standard model [1]. In the frame of the QSNET project [2], we are setting up a molecular lattice clock to test for time-variation of the proton-to-electron mass ratio. The clock will be based on the fundamental vibrational transition in Calcium Monofluoride (CaF) at a wavelength of around 17µm. The transition is expected to have a sub-Hz linewidth and be largely insensitive to systematic DC Stark or Zeeman shifts. Additionally, the AC Stark shifts of the ground and excited states of the clock transition are expected to cancel for several wavelengths, potentially facilitating the trapping of the molecules in a magic wavelength lattice [3]. The frequency of the clock transition is currently known to several MHz. To narrow this down, we will perform vibrational spectroscopy of magneto optically trapped CaF with a 17µm quantum cascade laser (QCL) [4]. The frequency of the QCL will be referenced to absorption lines of the v2 fundamental vibration mode of N_2O in the 17µm region. We measure these, for the first time, with frequency modulation spectroscopy and linearize the QCL frequency scan with a cavity.

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B6-4-HT

The origin of enhanced O_2^+ production from photoionized CO_2 clusters

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Clusters studies improve our fundamental understanding of the evolution of matter from a single molecule to an infinite solid. Recent quantum chemical calculations predict that pure CO_2 clusters exist at high altitudes in the CO_2-rich Martian atmosphere as cloud precursors [1]. Interaction of light with atmospheric particles is ubiquitous. At these high altitudes (60-100 km), ionizing radiation is abundant and can induce dissociation reactions in CO_2 clusters. While the formation of O_2^+ after X-ray ionization of CO_2 clusters has been previously reported [2], we present here a comprehensive experimental and theoretical study on the underlying mechanisms that lead to the production of O_2^+ [3].

We investigate the production of O_2^+ from core-ionized CO_2 clusters, using 3-D momentum coincidence imaging. CO_2 clusters were ionized using soft X-Rays (320 eV) from the MAX-II storage ring in Lund, Sweden. The measured O_2^+ yield from the ionized CO_2 clusters is substantially higher than molecular studies [4] as shown in Figure 1. The dramatic increase in yield is due to the presence of intermolecular interactions in clusters, that opens specific reaction pathways. The ion-momentum analysis shows that O_2^+ ions are produced via two different sequential dissociation processes in the clusters; and these are dependent upon the cluster size.

Quantum chemical calculations allow us to propose different reaction pathways. The simulations show that the most efficient photoreaction leading to O_2^+ is when the mother cluster ion has an icosahedral structure. We believe that these reactions are relevant to the chemistry of the CO_2-rich Martian atmosphere and can contribute to the O_2^+ concentration in the ionosphere [5].

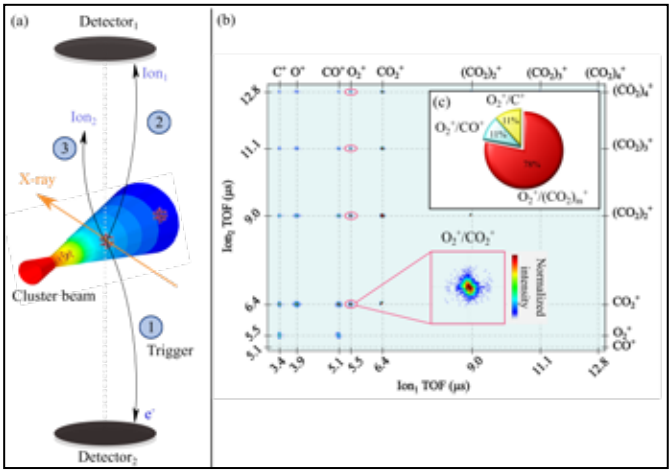

Figure 1. (a) A schematic of the experiment showing a typical double coincidence measurement. Detector$_1$ measures 3-D momentum of the ions. (b) 2-D coincidence map of time-of-flights (TOFs) of ions produced by CO_2 clusters at mean size of 20 molecules ionized by X-ray photons (320 eV). All the cluster dissociation channels producing O_2^+ ions are highlighted in red. (c) Contribution of the different dissociation channels to the overall O_2^+ production from clusters.

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Realizing a topological gauge theory in an optically dressed Bose-Einstein condensate

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Topological gauge theories describe the low-energy properties of certain strongly correlated quantum systems through effective weakly interacting models. A prime example is the Chern-Simons theory of fractional quantum Hall states, where anyonic excitations emerge from the coupling between weakly interacting matter particles and a density-dependent gauge field. While in traditional solid-state platforms such gauge theories are only convenient theoretical constructions, engineered quantum systems enable their direct implementation and provide a fertile playground to investigate their phenomenology without the need for strong interactions. In my talk, I will present the quantum simulation of a one-dimensional reduction of the Chern-Simons theory, the chiral BF theory, in a Bose-Einstein condensate [1,2]. Using the local conservation laws of the theory we eliminate the gauge degrees of freedom in favor of chiral matter interactions, which we engineer by synthesizing optically dressed atomic states with momentum-dependent scattering properties. This allows us to reveal the key properties of the chiral BF theory: the formation of chiral solitons and the emergence of an electric field generated by the system itself. Our results expand the scope of quantum simulation to topological gauge theories and pave the way towards implementing analogous gauge theories in higher dimensions.

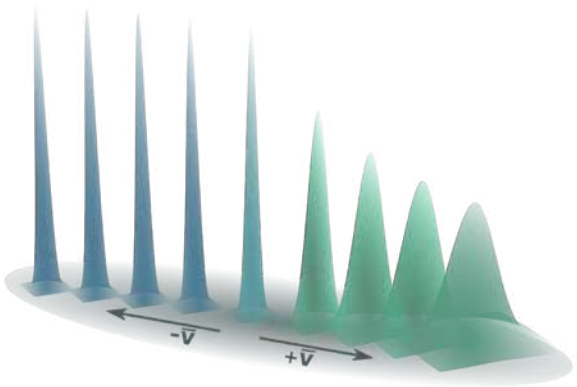

FIG. 1: Artistic view of a chiral Bose-Einstein condensate realizing the chiral BF theory.

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A7-2-INV

Speeding up a trapped ion quantum processor via Rydberg interaction

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Trapped Rydberg ions are a novel approach for quantum information processing [1,2]. This idea joins the advanced quantum control of trapped ions with the strong dipolar interaction between Rydberg atoms. For trapped ions, this method promises to speed up entangling interactions and to enable such operations in larger ion crystals.

In this presentation, I will introduce the novel experimental platform of trapped Rydberg ions [2]. I will describe the specific physics involved when exciting ions into Rydberg states, the effects on the trapping potential due to the strong polarizability of Rydberg ions, and the controllable strong interaction between ion and motion. Moreover, I will summarize methods and results in speeding up trapped ion entanglement operations via strong dipolar Rydberg interaction [3].

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Mott-squeezed states with ultra-cold fermions

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I will present our recent work [**1**] where we consider dynamical generation of spin squeezing in a lattice system composed of ultra-cold fermionic atoms in the Mott phase at half filling. The initial spin coherent state does not change in time during unitary evolution under the Fermi-Hubbrd Hamiltonian. In order to induce the generation of squeezing we add the position-dependent laser coupling between internal degrees of freedom of atoms [**2**]. We study the Ramsey-type spectroscopy scheme in which the atom-light coupling is turned on during the interrogation time, as illustrated in Fig. 1. We show analytically, using the perturbation theory, how the Fermi-Hubbard model with the atom-light coupling effectively simulates the one-axis twisting model with tunable axis of squeezing. This paves the way for the simulation of the famous two-axis counter-twisting model when two laser couplings are used during the interrogation time. To illustrate and demonstrate the validity of our analytical finding, we perform full many-body calculations for several atoms taking into account periodic and open boundary conditions.

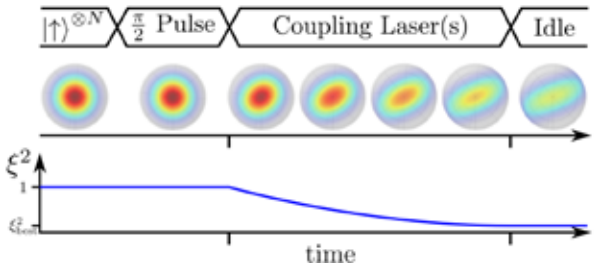

Figure 1: The Ramsey-type spectroscopy for the generation of Mott-squeezed states: (*i*) preparation of the initial spin coherent state with ultra-cold fermions in the Mott phase, (*ii*) unitary evolution using the Fermi-Hubbard Hamiltonian with the atom-light coupling reduces the value of the spin squeezing parameter ξ^2, (*iii*) freezing the spin squeezed state in the Mott phase when the atom-light coupling is turned off.

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Rydberg molecules : spectra and scattering properties

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Ultralong-range Rydberg molecules are formed by exciting a Rydberg atom in a ultracold gas of atoms. At a high density of ultracold gas one or more ground-state atoms can be found within the Rydberg electron wavefunction. Even with a weak interaction between the Rydberg electron and a ground-state atom, the ground-state atoms can be bound to the Rydberg atom at low temperature to form a Rydberg molecule. For Rydberg dimers created using strontium atoms, the vibrational ground state has a well defined bond length which can be controlled by the principal quantum number n of the Rydberg electron (Fig.1). This feature can be used to extract different information on the scattering between two atoms from the photoassociation spectra of Rydberg molecules. In particular, strontium is suitable for such studies having several stable isotopes with different scattering characteristics.

Since the excitation of the ground vibrational state reflects the probability to find a pair of initial ground-state atoms whose separation is close to the bond length, the excitation strength of a Rydberg dimer with different values of n can be mapped to a pair correlation function of the initial ultracold gas [1]. By exciting the Rydberg electron up to $n = 40$, the pair correlation can be probed to the long length scale ($\sim$ 3000 a.u.) which is on the order of de Broglie wavelength at 1 μK. A comparison of bosonic (^{84}Sr) and fermionic isotopes (^{87}Sr) reveals the effects of quantum statistics (Fig.2). The excitation strength is also sensitive to the scattering length between ground state atoms. For ^{86}Sr, the s-wave scattering length is 811 a.u. which is close to the bond length of $n = 25$ Rydberg dimer. Therefore, around $n = 25$ the contributions of s-waves to the Rydberg molecule excitation spectra are largely suppressed and, instead, the excitation of rotational levels can be pronounced. This can be used to probe the effect of recoil momentum by photon absorption. Unlike typical homonuclear dimers, Rydberg molecules are very asymmetric. A photon absorption boosts only one of the atoms and transfers the rotational angular momentum to the dimer. Due to the long bond length, a small recoil momentum can transfer a sizable angular momentum to the molecule [2].

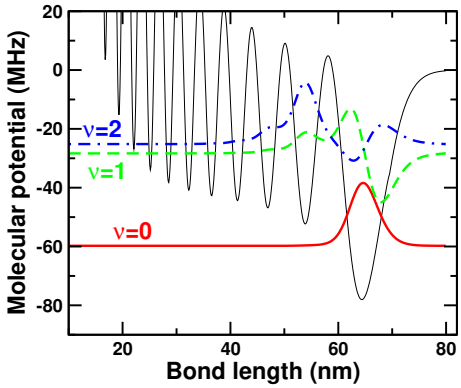

FIG. 1: Molecular potential for a strontium Rydberg dimer. The vibrational wavefunctions for the $\nu = 0, 1$, and 2 vibrational states are also included and the horizontal axis for each shows its binding energy.

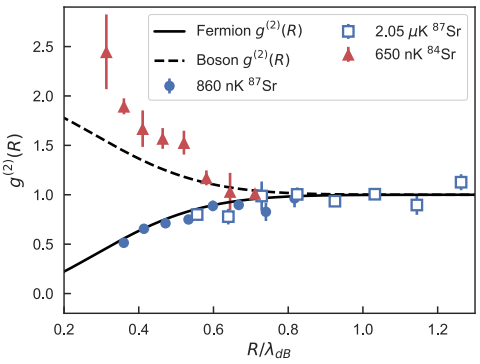

FIG. 2: Pair correlation $g^{(2)}(R)$ for Fermi and Bose gases as a function of internuclear distance scaled by the thermal de Broglie wavelength. $g^{(2)}(R)$ for ideal gases are also shown.

This work is a collaboration with Y. Lu, R. Ding, J. D. Whalen, S. K. Kanungo, T. C. Killian, F. B. Dunning (Rice Univ.), M. Wagner, R Schmidt (Max-Planck-Inst.), H. R. Sadeghpour (ITAMP) and J. Burgdörfer (Vienna Univ. of Technology).

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B7-1-INV

X-rays from the Universe

Joern Wilms

Most of what we know today about the properties of the hot and energetic universe has been learned using observations with X-rays from satellites. These observations have permitted, e.g., to measure the properties of black holes which accrete material from their surroundings or to determine the state of the plasma in the remnants of supernova explosions or in the gas between galaxies in galaxy clusters. X-ray astronomical measurements rely on the precise knowledge of the properties of inner shell transitions in (often highly ionized) elements heavier than hydrogen or helium. The talk will give an overview of some of the recent results in X-ray astronomy and discuss the data needs for the next generation of X-ray astronomical missions such as the microcalorimeters on the Japanese-American XRISM mission, which is to be launched in 2023.

Ultrastable frequency transfer through optical fiber links at the continental scale

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Optical fiber links enable the accurate and ultra-stable transfer of an optical frequency reference for the comparison of distant optical clocks and for a wide range of precision measurements. In France, a wide scale fiber network, called REFIMEVE, has been developed, using the academic network of RENATER. It aims to disseminate ultra-stable and accurate time and frequency signals generated at LNE-SYRTE to around thirty partner laboratories at the national scale and to connection points to European National Metrological Institutes. The network is currently composed of four national-scale links and three regional links, for a total of 2×2600 km and it disseminates an accurate frequency signal with a residual transfer uncertainty better than 10^{-19}. It is highly reliable and robust thanks to regeneration stations installed along the network, which provide both remote control and real-time supervision [1,2].

REFIMEVE is part of the fiber links enabling the accurate comparison of a wide set of European atomic clocks, which benefits to fundamental metrology and can be applied to chronometric geodesy or search for new physics. Moreover ultra-stable frequency transfer also currently benefit to high-resolution spectroscopy, remote laser control, photonics or Earth sensing. A few example of applications will be shown at the conference, among them precision molecular spectroscopy in the mid-infrared using Quantum Cascade Lasers [3].

FIG. 1: Map of the REFIMEVE network and its European connection.

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Towards stimulated decay of antihydrogen atoms

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Several experiments at CERN's antiproton decelerator produce antihydrogen atoms via various mechanisms leading to formations in Rydberg states. When held in a magnetic trap the antihydrogen atoms can spontaneously decay to their ground states from which high precision spectroscopy measurements can be realized. Comparisons with hydrogen values allow for stringent tests of the CPT symmetry, a fundamental pillar of quantum field theory.
Beam experiments, which have been proposed to measure with high precision the antihydrogen ground state hyperfine splitting or the effect of gravity on antimatter atoms, cannot currently rely on the too slow spontaneous decay to populate the ground state, and hence need alternative mechanisms to deexcite the atoms.
I will present recent ideas to reduce by several orders of magnitude the lifetime of the initially populated levels [**1**, **2**] and give an overview of a proof-of-principle hydrogen deexcitation experiment being developed [**3**] to test them. I will also shortly address potential applications of stimulated deexcitation in trap experiments for enhanced trapping and cooling [**4**].

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An Apparatus for the Production of Squeezed Momentum State Superpositions in Atom Interferometers

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Atom Interferometry for gravity measurements is now approaching its precision limits set by the Standard Quantum Limit (SQL) of phase estimation [1]. Within the bounds of the SQL, the minimum statistical uncertainty in gravity measurements scales as $1/\sqrt{N}$, where N is the number of atoms entering the interferometer. Quantum entanglement is an important resource that can potentially improve this scaling with atom number and therefore the sensitivity of atom interferometers beyond classical limits. In this context I will present a recently developed apparatus for the production of entangled squeezed states of strontium atoms that can be injected in a matter-wave interferometer with separated arms. The core of the apparatus is a high-finesse optical ring cavity (shown in Fig. 1) conceived in order to induce strong collective coupling between the atomic ensemble and the cavity mode. I will show that this setup allows optical and atomic access for interferometer operation and that it allows for homogeneous atom-light interaction. This setup will enable the production of squeezed states either by quantum nondemolition measurement or by deterministic protocols such as one-axis twisting [2]. It will allow to test the proposal [3] for the production of squeezed momentum state superpositions for atom interferometry.

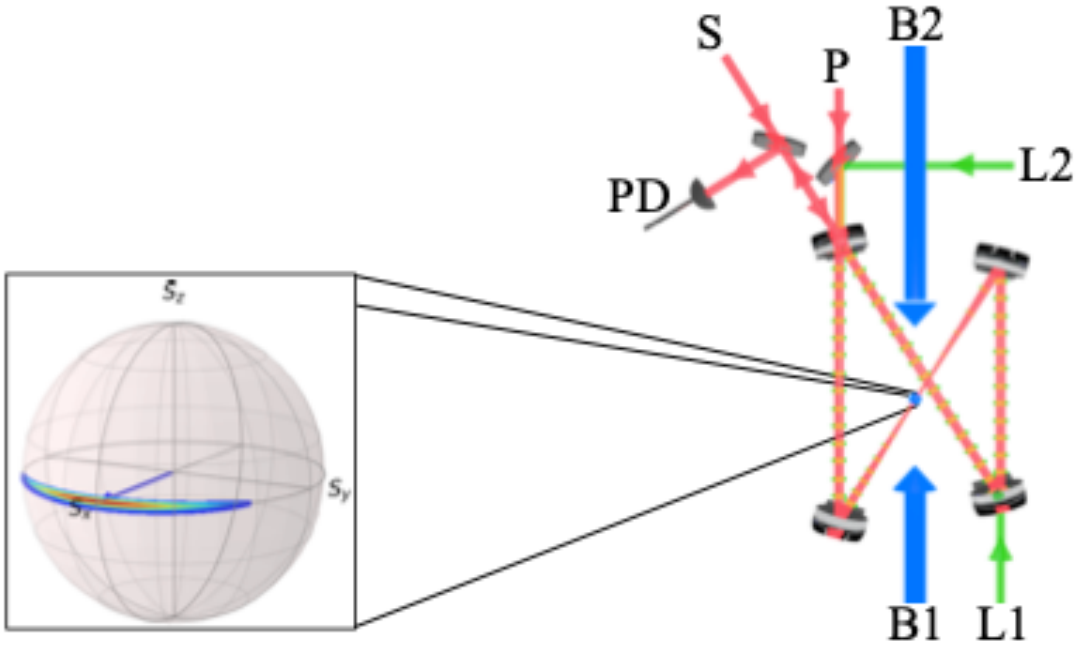

FIG. 1: Schematic illustration of the setup with the high-finesse optical ring cavity coupled to a squeezed atomic ensemble. Optical lattice beams (L1,L2) for atom trapping, interferometry beams for Bragg diffraction (B1,B2), the probe beam (P) and the cavity stabilization beam (S) are shown. The inset shows the squeezed state representation in the Bloch sphere.

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The European Research Council – funding opportunities for bright minds

Christian Oswald

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Is an ERC grant for you? I will explain what the European Research Council is, who can benefit from its funding opportunities and what to expect in the application and selection process. I will focus on the grants for early-career researchers (up to 12 years after PhD). The ERC supports researchers performing interesting and ambitious fundamental research. This could be you.

The mission of the European Research Council is to encourage the highest quality research in Europe. The concept is simple, competitive individual funding for researchers with a great idea, across all fields. ERC grants are awarded through open competition to projects headed by starting and established researchers of any nationality and age, who are working or moving to work in Europe or an associated country. The sole criterion of choice is scientific excellence. The ERC approach allows researchers to identify new opportunities and directions in any field of research, rather than being led by set priorities. This ensures that scientists are the ones driving the development of their field.

Hybrid GaSb/Si spectroscopic sensing technology as a generic technology platform for next-generation IoT and health applications

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Infrared spectroscopy is an established platform for a large variety of different spectroscopic sensing applications – from food industry, through chemical industry to law enforcement. However, most of the applications are limited as off-site/off-line laboratory measurement, as the typical spectroscopic system size is that of a table-top instrument and the prices is in the tens of thousands of EUR, limiting wider adoption. Semiconductor technology has been driving the technology revolution and acted as the key-instrument in widespread of technology to a wide audience – from personal computers, to internet and smartphones mainly due to the advancement in integrated circuit technology and optoelectronic components. Silicon photonics, when combined with the right III-V semiconductor, maybe the next revolution driver, in particular in the field of spectroscopic sensing, offering a unique opportunity to transfer the off-line/off-site lab instrument to in-line/ on-site and real-time instrument, providing continuous stream of data directly from the process of interest. We demonstrate a spectroscopic platform for accessing 1st overtone and combination band molecular absorption due to the vibrations of different C-H, O-H, N-H bonds and their combinations [1]. This band offers higher molar absorptivity, and, most importantly, specificity when it comes to complex objects under the experiment. From hardware point-of-view, the technology has to be scalable, room-temperature operational and sufficiently low cost to support the scale-up from the lab to the field. At BROLIS, we develop a spectroscopic platform based on hybrid integration of type-I GaSb gain-chip with silicon based photonic integrated circuit and also GaSb based photodetector. Photonic integration circuit acts as light manipulation platform for optical feedback, wavelength, power and phase control, tuning, locking and monitoring. GaSb gain-chip acts as an active optical amplifier and together with the PIC form an external cavity widely tunable laser, whereas the GaSb photodetector is used for both internal and external signal monitoring. Such system has no moving parts and is controlled electronically (Fig.1).

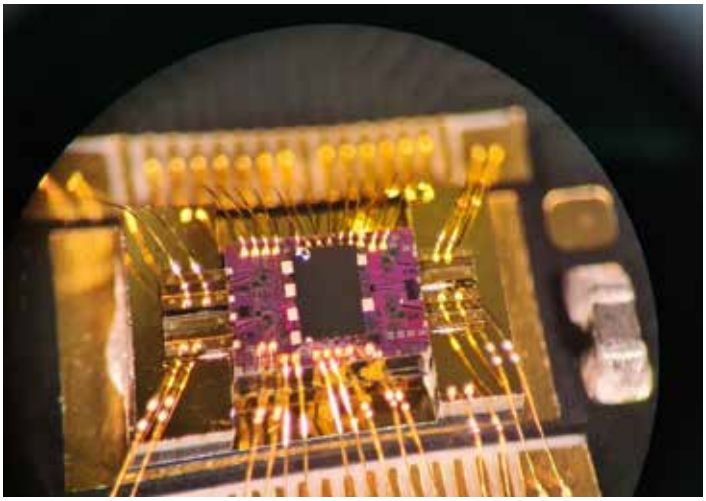

FIG. 1: Brolis GaSb/Si 4-channel laser spectrometer-on-a-chip.

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Career Opportunities in the Scientific and Industrial Laser Technologies

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Lasers and photonics became keywords describing the high-tech industry in Lithuania. Starting from the early years after laser discovery, Lithuania's laser sector has grown into a fully self-sustaining ecosystem that is built on tight connections among research entities and companies.

As most – and at the beginning nearly all – employees of Lithuanian laser manufacturers had their start in laser physics at Vilnius University, the relationship between academia and industry in this sector has always been strong. This close relationship facilitated to laser solutions that are unique in the global market.

For young researchers are two ways to join. One is to transform your knowledge into new products and solutions for companies, staying as a researcher or moving from research carrier to business. If you fill having a sense of entrepreneurship, you can establish a spin-off company trying to implement your PhD research finding and ideas into new services and innovative products.

Being in a close collaborating community helps to test yourself and find a position which is more appropriate to your wishes and habits: optics, lasers, applications, services or teaching.

Discover Modern Trends in Optoelectronics Research at FTMC: Materials, Technology and Applications for Terahertz Photonics

Gintaras Valušis

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Terahertz (THz) range covers the electromagnetic radiation spectrum from 1011 Hz to 1013 Hz frequencies with corresponding energies are 0.4–40 meV, falling hence between the millimeter waves and the infrared range. Sometimes is is called „*THz gap*“ as, in regard to device physics, from the „*red side*“, it is the energy region between a classical carrier transport with the cut-off frequency defined mainly by carrier transit time or parasitic RC time constants, and, from the „*blue side*“, it is defined by quantum mechanics rules governed photonic devices. Therefore, technology of devices and their applications in this range requires nonconventional approaches and specific solutions.

In this talk, we discuss principles, materials designs and technology for development of compact TH imaging and spectroscopic systems [1]. Principles of emitters and detectors operation will be discussed, special attention will be dedicated to the design of flat optics components.

Modern trends in THz optoelectronics and photonics as well as scientific challenges will be revealed.

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Recent Developments of NIST Atomic Databases and Online Tools

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The National Institute of Standards and Technology (NIST) has an active research program on atomic spectroscopy that includes precise measurements (e.g., Fourier Transform spectroscopy of neutral and low-charged ions as well as spectroscopy of highly charged ions with electron beam ion traps), theoretical calculations with various non-relativistic and relativistic atomic structure methods, development and expansion of atomic databases of recommended physical reference data, and development of online tools for calculation of plasma spectra (see, e.g, [1]). The most extensive database of recommended spectroscopic data, the NIST Atomic Spectra Database (ASD) version 5.9, currently provides critically evaluated data on more than 112,000 energy levels, 291,000 spectral lines, 122,000 transition probabilities, and 6000 ionization potentials for elements from H (Z=1) to Ds (Z=110) (see Fig. 1 for a complete coverage for spectral lines). In this talk I will describe the recent developments of the NIST atomic databases including, in particular, upgrades of and data additions to ASD, status of the Laser-Induced Breakdown Spectroscopy (LIBS) spectrum-generation tool, the recently developed NIST-LANL Lanthanide Opacity database for kilonova modeling, and the collisional-radiative code FLYCHK.

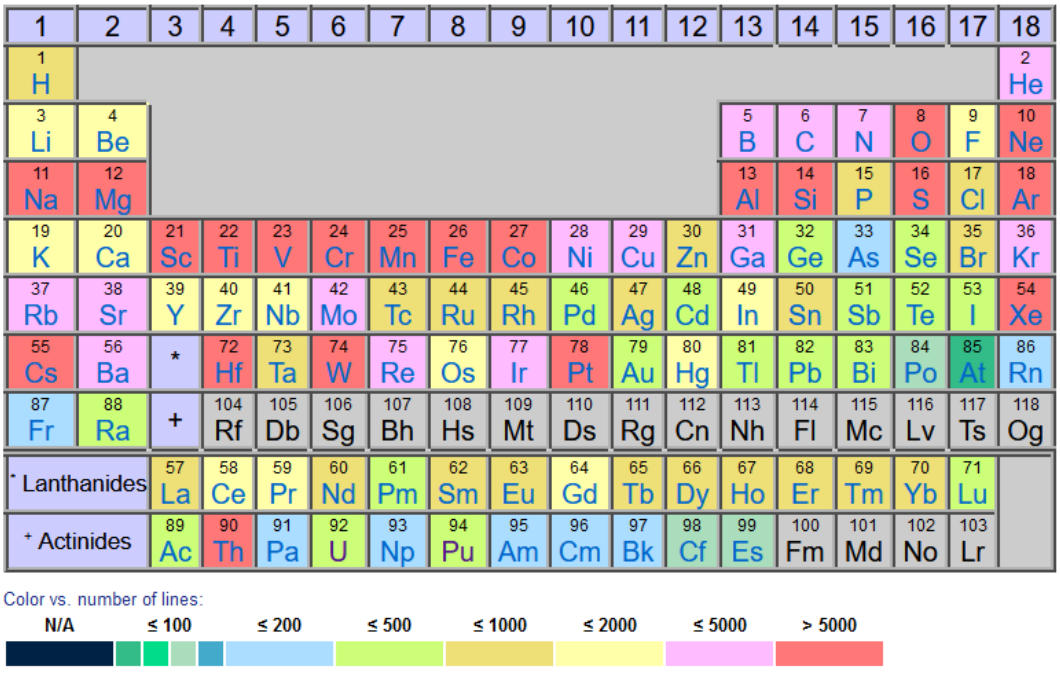

Figure 1. Contents of ASD for spectral lines (v.5.9). Different colors represent the number of spectral lines for different elements.

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Magnetometry with a nanometric-thin K vapor cell

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Alkali atoms are commonly used in atomic physics for a number of reasons, the main one being the simplicity of their electronic structure. Relatively cheap lasers are available for the main optical transitions (D lines) of most alkali atoms making them convenient to study experimentally, mainly in the domain of magnetometry [1, 2]. Potassium 39 (^{39}K) is an interesting candidate for such experiments, since it has the smallest characteristic value $B_0 = A_{^2S_{1/2}}/\mu_B \approx 170$ G (where $A_{^2S_{1/2}}$ is the ground state's magnetic dipole interaction constant) characterizing the decoupling of **J** and **I** and therefore the establishment of hyperfine Paschen-Back (HPB) regime [3, 4]. Probing a ^{39}K vapor with a circularly polarized laser while applying a strong enough (> 200 G) magnetic field oriented along the propagation direction of laser allows to record an absorption spectrum in which only 8 spectrally resolved Zeeman transitions (4 for each circular polarization $\sigma^{\pm}$) are visible, while the probabilities of the 16 remaining transitions tend to zero. Complete spectral resolution is obtained thanks to the thickness of the vapor cell, allowing almost complete cancellation of the Doppler broadening [5]. We present a method that allows to measure the magnetic field with micrometer spatial resolution based on the recorded spectra in the range $0.1 - 10$ kG with a cell of thickness $L = 120 \pm 5 - 390 \pm 5$ nm, which is relevant in particular for the determination of magnetic fields with a large gradient (up to 3 G/μm). The experimental results are verified by theoretical calculations.

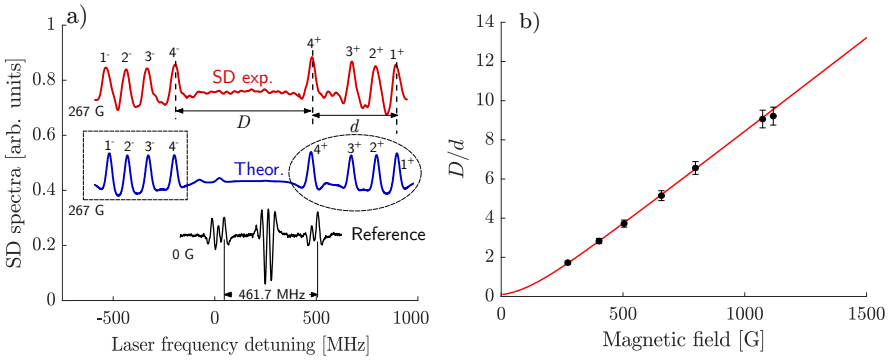

FIG. 1: a) ^{39}K D_1 line spectra recorded for $L = 385$ nm. Upper curve: experimental SD absorption spectrum for σ^+ and σ^- radiation recorded for $B = 267$ G. Middle curve: theoretical SD absorption spectrum. Lower curve: SD of a saturated absorption spectrum for reference. b) b) D/d as a function of the magnetic field. Solid line: theory. Dots with error bars: experimental measurements, the inaccuracy is 5%.

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Competitive Dehydrogenation and Backbone Fragmentation of Super-Hydrogenated PAHs

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Super-hydrogenated Polycyclic Aromatic Hydrocarbons (PAHs) have been suggested to catalyze the formation of H_2 in certain regions of space, but it remains unclear under which circumstances this mechanism is viable given the reduced carbon backbone stability of super-hydrogenated PAHs [1, 2, 3]. We report a laboratory study on the stability of the smallest pericondensed PAH, pyrene ($C_{16}H_{10+N}$, with $N = 4$, 6, and 16 additional H atoms, see Fig. 1), against photodestruction by single vacuum ultraviolet photons using the Photo-Electron Photo-Ion Coincidence (PEPICO) technique [4]. For 4H-Pyr ($N = 4$), we observe a protective effect of hydrogenation against the loss of native hydrogens. No such effect is seen for 6H- or 16H-Pyr, where the weakening effect of replacing aromatic bonds with aliphatic ones outweighs the buffering effect of the additional hydrogen atoms. In all three cases, H-loss and C_mH_n-loss ($m \geq 1$, carbon backbone fragmentation) channels open at approximately the same energy. The branching fractions of the primary channels favor H-loss for 4H-Pyr, C_mH_n-loss for 16H-Pyr, and are roughly equal for the intermediate 6H-Pyr. Figure 1 shows the branching fractions of the first few fragment groups from the PEPICO measurement at a common electron binding energy of 13.6 eV, corresponding to the highest photon energy expected to impinge on PAHs in photodissociation regions. We conclude that super-hydrogenated pyrene is probably too small to support catalytic H_2-formation, while trends in the current and previously reported data suggest that larger PAHs may serve as catalysts up to a certain level of hydrogenation [4].

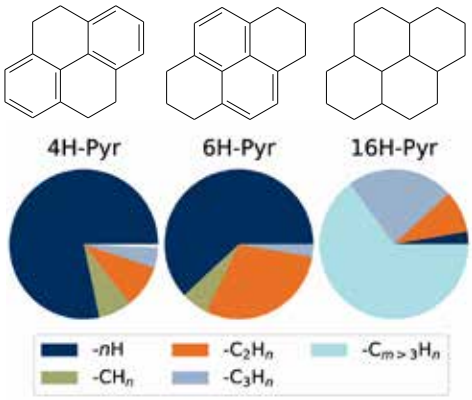

FIG. 1: Structures of 4H-, 6H-, and 16H-Pyr. Comparison of the branching fractions of the first few fragment groups at a binding energy of 13.6 eV.

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POSTER ABSTRACTS

SESSON 1

Revealing exciton Hamiltonian of Chlorophyll aggregate from 2DES crosspeak region

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Frenkel exciton Hamiltonian has been extensively used for describing electronic spectra of molecular complexes of an arbitrary size and geometry [1]. Determination of the Hamiltonian parameters, molecular excitation energies and inter-molecular interactions, has always been a big challenge. Molecular nonlinear spectroscopy has been used as a tool for this purpose. There are various theoretical methods to describe exciton nonlinear spectra, however, inversion of the problem is usually not straightforward due to exciton delocalization and spectral broadening.

Crosspeak region of the two dimensional electronic spectra (2DES) is very sensitive to intermolecular couplings, however the obtained information on exciton Hamiltonian is very indirect [2]. We suggest that specific local molecular excitations, that are separated from main exciton band can be additionally employed to dramatically enhance resolution and directly reveal exciton Hamiltonian. This proposed scenario can be directly applied to Chlorophyll aggregates since Chlorophylls have two perpendicular molecular transitions, usually denote by Qy and Qx. Since Qx transitions are localized, they are used to obtain information on exciton wavefunctions and exciton composition in Qy region. The scheme is described in terms of double-sided Feynman diagrams and demonstrated on a realistic model Chlorophyll dimer (Fig. 1). Molecular excitation energies, intermolecular couplings and exciton compositions are directly revealed as specific peak splitting and their amplitude variations in YX crosspeak region of the 2DES spectra.

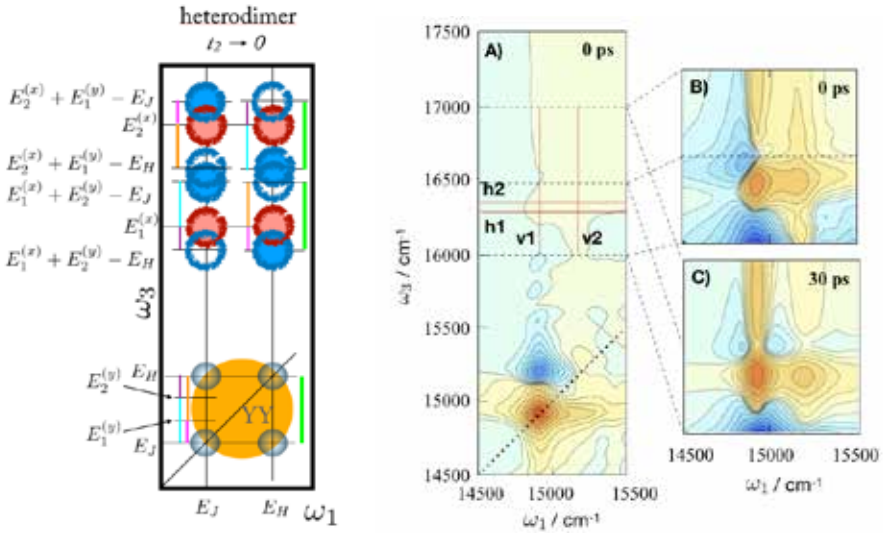

FIG. 1: 2DES spectrum of a Chlorophyll dimer in broad band region covering Qy and Qx excitations. Left: peak pattern of a generic Chlorophyll dimer. Right: A - calculated 2DES spectrum of the dimer with realistic parameters, B, C – crosspeak region.

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Retinal Imaging with Fourier-Domain Full-Field Optical Coherence Tomography and a Multimode Fiber for Coherence Noise Reduction

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Optical coherence tomography (OCT) is an interferometric imaging method – widely used for retinal imaging – that can image deep in tissue. Full-field OCT (FF-OCT) is an OCT variant that uses a CMOS camera instead of a single point detector, which eliminates the need to scan sample in both *x* and *y* directions, and achieves higher lateral resolution [1]. By employing Fourier-domain data acquisition method (via utilization of a tunable narrowband light source) and an ultrafast CMOS camera, FF-OCT becomes a fast imaging modality, suitable for in vivo human eye imaging [2]. However, crosstalk appearing from use of a spatially coherent laser (and widefield detection) has been limiting the technique's performance, preventing from seeing choroid and other retinal layers. It is important to image choroid in human eye as it is a crucial determinant in the pathogenesis of many ocular diseases, since its principle role is to supply oxygen to the outer retina [3]. A spatially incoherent light source can be used to remove crosstalk, as was shown previously by the help of an ultrafast deformable membrane [4]. Here we show that using a multimode fiber with carefully chosen parameters [5] the entire thickness of the retina and choroid can be acquired in one volume *in vivo* with suppressed crosstalk and high contrast [6], as shown in Fig. 1. This implementation can speed up the clinical adaptation of FF-OCT technology.

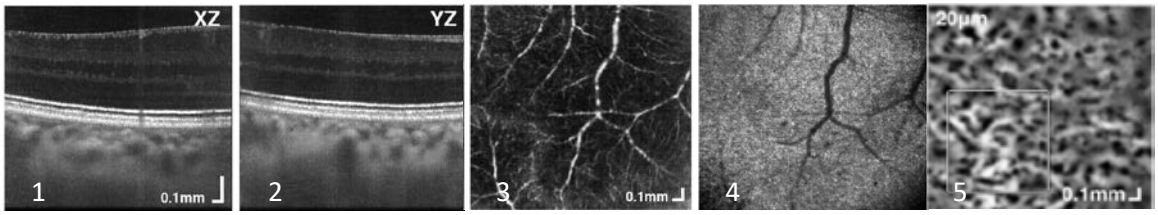

FIG. 1: FF-OCT images of a retina acquired in less than 0,1s. Axial views (1, 2) and *en face* views (3,4) of the retina and choroid (5), which were derived from the acquired retinal data, shows high resolution and high contrast.

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Vacuum Magnetic Birefringence: an Optical Test of Quantum ElectroDynamics

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The BMV (*Biréfringence Magnétique du Vide*) project is an ambitious experiment whose goal is to verify in the laboratory the vacuum energy predictions of Quantum ElectroDynamics (QED). This theory predicts that the vacuum, in the presence of a magnetic field, behaves like a birefringent medium. The experiment mixes intense pulsed magnetic fields with a sensitive optical device, centered around a high finesse Fabry-Perot cavity.

In the presence of a transverse magnetic field, a linearly polarized light will become elliptically polarized and acquired an ellipticity Ψ expressed as

$$\Psi = \frac{2\mathcal{F}L_B}{\lambda}\Delta n \tag{1}$$

where L_B is the magnetic region length, $\mathcal{F}$ the cavity finesse and Δn the difference of index of refraction induced by the field. It can be expressed as $\Delta n = k_{\mathrm{CM}}B^2$ with $k_{\mathrm{CM}} = 4\times10^{-24}$ T^{-2} is the QED prediction for vacuum. Thus, achieving this measurement would allow to directly test QED in the photonic sector.

Since the last published BMV data run in vacuum, a Monte Carlo simulation of the experiment gave insights on the origins of the optical noise of our experiment. More recently we commissioned a new unique pulsed field magnet and with the lessons learned from our noise studies it allowed us to reach our best limit yet with room for further improvements.

I will present our experiment and its challenges as well as our latest results.

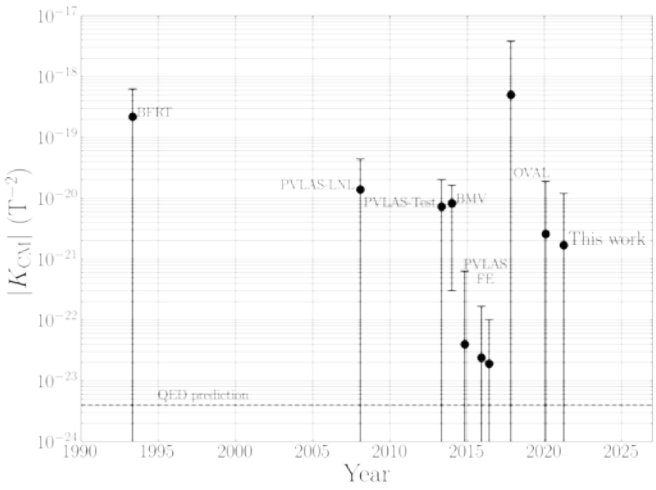

Figure 1: Published measured values of vacuum magnetic birefringence by different experimental groups across the years, errors bars are represented with a coverage factor $k = 3$.

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Dimensional crossover in the superfluid-supersolid quantum phase transition in an elongated dipolar condensate

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We provide a theoretical description of the superfluid-supersolid phase transition for a dipolar condensate confined in an elongated trap, as observed in the recent experiment by G. Biagioni *et al.* [Phys. Rev. X , (2022)]. By means of the extended Gross-Pitaevskii theory, which includes the Lee-Huang-Yang quantum fluctuation term, we analyze the ground state configurations of the system as a function of the interparticle scattering length, for two different trap configurations. We show that for sufficiently strong confinement the transition has a smooth (continuous) character, whereas for shallower transverse traps a discontinuity clearly shows up.

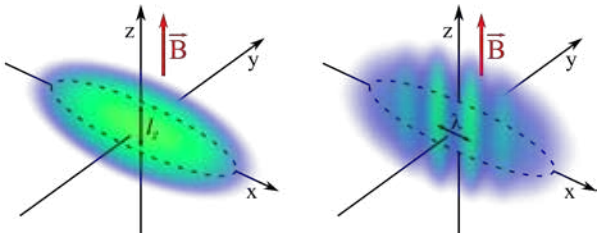

FIG. 1: Condensate configurations in the superfluid and supersolid phases.

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Magnetic field values cancelling alkali atoms' transitions

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Analytically, all electric dipole transitions (π, σ^+ and σ^-) between the magnetic sublevels of D_1 line of all alkali metal atoms are considered [1]. General 2×2 block Hamiltonian matrices corresponding ground and excited states are constructed. After the eigenkets and eigenvectors are calculated, we obtain "modified" transfer coefficients which depend on the nuclear spin I, the magnetic quantum number m and the magnetic field magnitude B. Transition cancellations exist only for some π transitions of each isotope where the total atomic angular momenta of ground and excited states are equal to each other ($F_g = F_e$). As a result, we obtain a unique formula which expresses the magnetic field values canceling these transitions:

$$B = -\frac{2m}{\mu_B(1+2I)} \times \frac{2\varepsilon_g\varepsilon_e}{(g_I - g_S)\varepsilon_e + \dfrac{3g_I - 4g_L + g_S}{3}\varepsilon_g}, \tag{1}$$

where μ_B is the Bohr magneton, m is the magnetic quantum number, I is the nuclear spin, g_I, g_S and g_L are respectively the nuclear, electronic and angular Landé factors, ε_g and ε_e are the energy difference of the ground and excited states, and $0 \leq (-1)^{2I} m \leq I - 1/2$. These B values also correspond to the case when some of other transitions intensity reach their maximum. Furthermore, we examine the derivative of π transition "modified" transfer coefficients in order to find the magnetic field values corresponding to the maximum transition intensities.

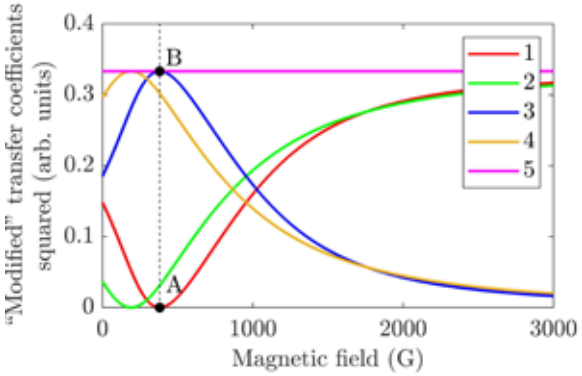

FIG. 1: ^{85}Rb D_1 line "modified" transfer coefficients squared. The vertical dashed line indicates the value $B = 380.73$ G which corresponds to the cancellation of the transitions (point A) and coincides with the maximum of transitions (point B). Lines 1 and 2 correspond to the transfer coefficients for $m = -2$ and $m = -1$ values respectively, where $F_g = F_e$. Lines 3 and 4 correspond to the transfer coefficients for $m = -2$ and $m = -1$ values respectively, where $F_g \neq F_e$. "Guiding" transition coefficient squared (line 5) corresponds to $m = -3$.

For matrices of dimension higher than 2×2, formulas exist but are heavy, thus we have performed numerical calculations. We have analyzed $5^2S_{1/2} \rightarrow 5^2P_{3/2}$ and $5^2S_{1/2} \rightarrow 6^2P_{3/2}$ transition cancellations of the ^{85}Rb and ^{87}Rb alkali metal [2,3].

The accuracy of the magnetic field B values is limited solely by the uncertainty of the physical quantities involved in our calculations.

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Enhancing spin polarization using attosecond angular streaking

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We use the R-matrix with time-dependence method [**1** − **4**] to investigate spin polarization of electrons ejected from the krypton atom by an angular streaking scheme. Through solution of the multielectron, semi-relativistic, time-dependent Schrödinger equation, we show that angular streaking produces strongly spin-polarized electrons. We find that the degree of spin polarization attainable using the angular streaking scheme exceeds that acheived using longer circularly polarized pulses. The degree of spin polarization increases with the Keldysh parameter, so that angular streaking — ordinarily applied to investigate tunneling — may be repurposed to generate strongly spin-polarized electron bunches. Additionally, we explore modifications of the angular streaking scheme that also enhance spin polarization.

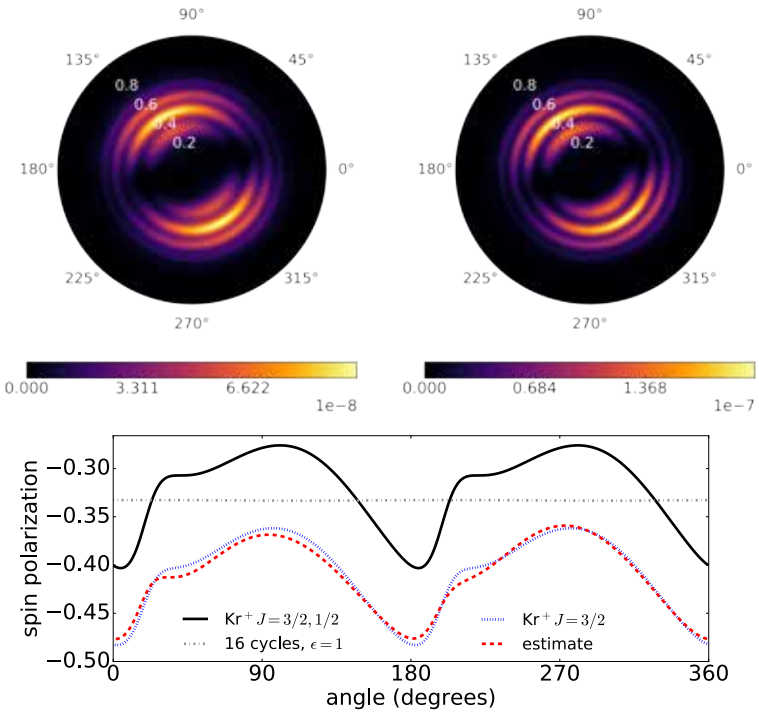

Figure 1: Momentum distribution for (a) spin up and (b) spin down electrons ionized from Kr by an 8-cycle, 780-nm, 2×10^{13} W/cm^2 pulse of ellipticity $\epsilon = 0.87$. (c) Momentum-integrated spin polarization, its dependence on the Kr$^+$ J value, and its single-threshold ($J = 3/2$) estimate.

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S1-P07

Theoretical study of photoelectron circular dichroism of a model chiral anion

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The forward-backward asymmetry in the emission of photoelectrons from randomly-oriented chiral molecules is known as photoelectron circular dichroism (PECD). For its quantitative description the differential photoionization cross-section with respect to the angle ϑ between the light propagation direction and that of photoelectrons outcome must be presented as an expansion over Legendre polynomials $P_l(\cos\vartheta)$:

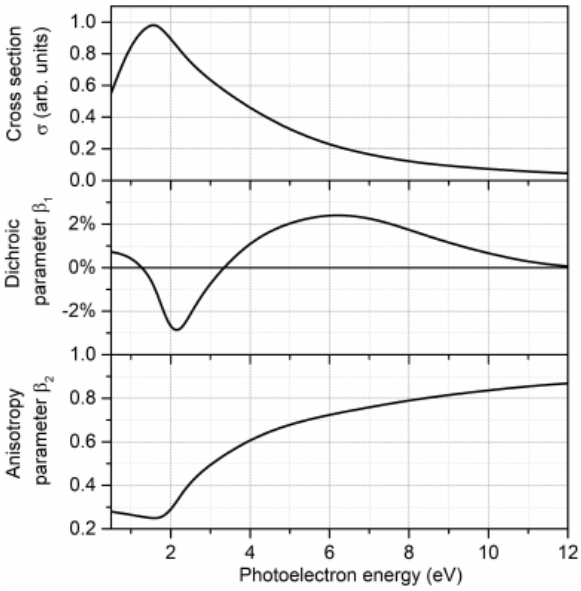
$$\frac{d\sigma^{\pm}(\vartheta)}{d\Omega} = \frac{\sigma}{4\pi}\left(1 \pm \beta_1 P_1(\cos\vartheta) - \frac{\beta_2}{2} P_2(\cos\vartheta)\right), \qquad (1)$$

where positive and negative signs correspond to the right or left circular polarization of laser, respectively, σ is the total cross-section; β_1 is known as dichroic and β_2 as anisotropy parameters.

The PECD was initially predicted by Ritchie [1] in one photon ionization of chiral molecule. He showed theoretically, that the PECD in photoionization of chiral molecules reveals itself already in the dipole approximation and can reach values of several percents for the dichroic parameter β_1. Later PECD in chiral systems was investigated in many other ionization regimes such as resonance-enhanced multiphoton ionization, above-threshold ionization, strong-field ionization, and multi-photon ionization by bichromatic fields. However, up to now only ionization of neutral molecules has been investigated.

In the present contribution we perform first theoretical study of PECD arising at the one photon ionization of model chiral anion molecule. For our investigations we use a model chiral system, similar to that used in Ref. [3] but with total charge $Z = -1$. Our investigations are stimulated by recent experiment by Krüger and Wetzel [2], where the sizeable (up to 4%) PECD was observed in photo-detachment of amino-acid anions.

Using time-dependent single center method [3-5] we calculated the photo-detachment of model chiral anion. In the figure one can see the plots of total cross-section as well as of both β parameters as a function of the incident photon energy [6]. It is clearly seen, that the β_1 as a function of photon energy changes its sign twice reaching at the maximum almost 3%, which agree very well with the results of Ref. [2].



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Interferometry on the Clock Transition in ^{87}Sr with Entangled Atoms in Momentum State Superpositions

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I will present our activity on the realisation of atom interferometry with an optical clock transition beyond the standard quantum limit (SQL) with strontium atoms. An interferometer can be injected with entangled atoms to improve its phase resolution $\Delta\phi$, where the entanglement is created between momentum state superpositions by performing cavity-enhanced quantum non-demolition (QND) measurements [**1**]. Our method will improves the scaling in phase resolution $\Delta\phi$ with atom number N surpassing the SQL of $\Delta\phi \sim N^{-1/2}$ for uncorrelated atoms. An interferometer using a similar method for entanglement creation has recently been demonstrated for a small atom number N and a short interrogation time T using rubidium atoms [**2**].

Atom interferometry can be used to study fundamental physics, like testing the equivalence principle or determining the gravitational constant G. It can furthermore be used in Earth observation sciences and in future space applications. To reach small phase resolutions $\Delta\phi$ interferometers need large-momentum transfer, a large atom number N and a long interrogation time T. However, many applications are limited by the size, weight and power consumption of the instrument, this is especially true for space applications. An interferometer implementing QND measurements can therefore be reduced in size, weight and power consumption compared to interferometers using uncorrelated atoms. Furthermore, when using squeezing a given precision is reached after a smaller averaging time, which improves the sensor bandwidth.

We plan to create an atom interferometer on the clock transition $^1S_0 \leftrightarrow {}^3P_0$ in strontium-87 [**3**] and inject it with entangled atoms using QND measurements. We realised a narrow-linewidth clock laser system at 698 nm to drive the clock transition. We are working on a homodyne detection system to perform the QND measurements. A momentum state superposition will be created between $\left|{}^1S_0, p = 0\right\rangle$ and $\left|{}^3P_0, p = \hbar k\right\rangle$ using single-photon transitions at 698 nm, with $\hbar k$ the momentum of a single photon. The QND measurements will be performed by probing the wave packets detuned from the $^1S_0 \leftrightarrow {}^3P_1$ transition at 689 nm when they cross the focus of the high-finesse experimental cavity (FIG. 1). Squeezing will be induced by measuring the populations in the prepared superposition. At the end of the interferometer sequence the population difference will be read out with increased sensitivity. This method can be used with other atomic species where a narrow transition is available or can be created.

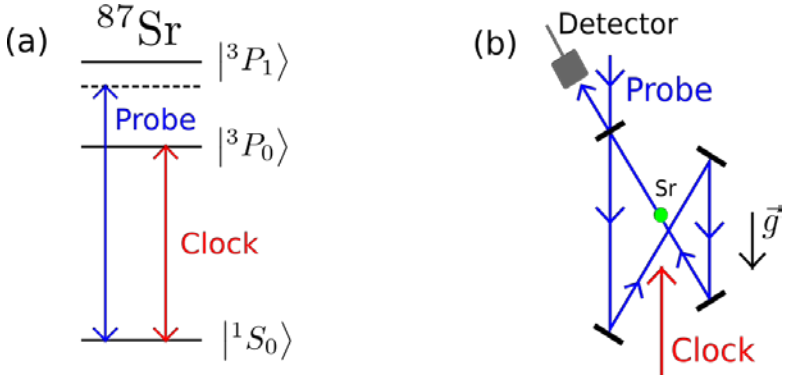

FIG. 1: (a) Simplified energy level diagram of strontium-87 (^{87}Sr). (b) Schematic representation of the probe beam (blue) coupled to the high-finesse cavity interacting with the Sr atoms (green circle). The interferometer pulses in free space (red) drive the single-photon transitions between momentum states.

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Chiral Rydberg States of Laser Cooled Atoms

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We propose a protocol for the preparation of chiral Rydberg states. It has been shown theoretically that using a suitable superposition of hydrogen wavefunctions, it is possible to construct an electron density and probability current distribution that has chiral nature [1]. Following a well established procedure for circular Rydberg state generation and subsequent manipulation with taylored radio frequency pulses under the influence of electric and magnetic fields, the necessary superposition of hydrogen-like states with correspondingly adjusted phases can be prepared. Enantio-selective detection using photo-ionization circular dichroism is under theoretical and experimental development

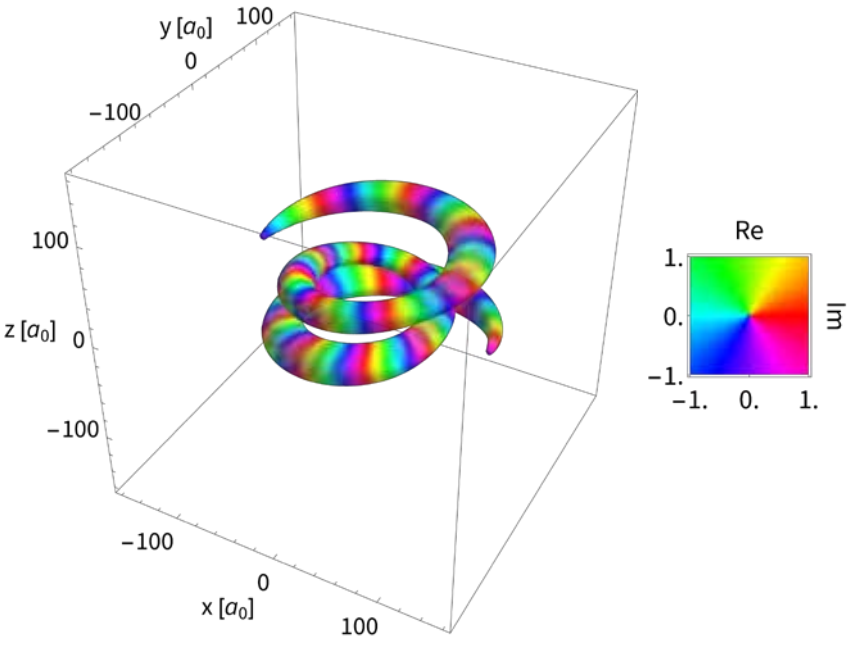

FIG. 1: Contour plot of a Chiral superposition of hydrogenic wavefunctions with color coding for the quantum phase.

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Atom Interferometry with Thousand-Fold Increase in Dynamic Range

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Atom interferometry offers high sensitivity in measuring acceleration, gravitational fields and their gradients, and rotations. In addition to precision measurements, atom interferometers are a promising technology for field applications such as mobile gravity surveys and navigational systems. Such applications require operation in mobile, and potentially noisy, environments and measuring rapidly-changing, unknown signals.

The periodicity inherent to any interferometric signal entails a fundamental trade-off between sensitivity and dynamic range of interferometry-based sensors. Here, we develop a methodology for substantially extending the dynamic range of such sensors without compromising their sensitivity, stability, and bandwidth [1]. The scheme is based on simultaneous operation of two nearly identical interferometers, providing a moiré-like period much larger than 2π and benefiting from close-to-maximal sensitivity and from suppression of common-mode noise (Fig. 1).

We implement this scheme for extending the dynamic range of atom interferometers, and demonstrate an enhancement of over an order of magnitude in a single shot and over three orders of magnitude within a few shots, without compromising the sensitivity, stability, and bandwidth. We achieve this for both static and dynamic signals, further introducing a novel implementation of particle filtering signal processing to atom interferometry.

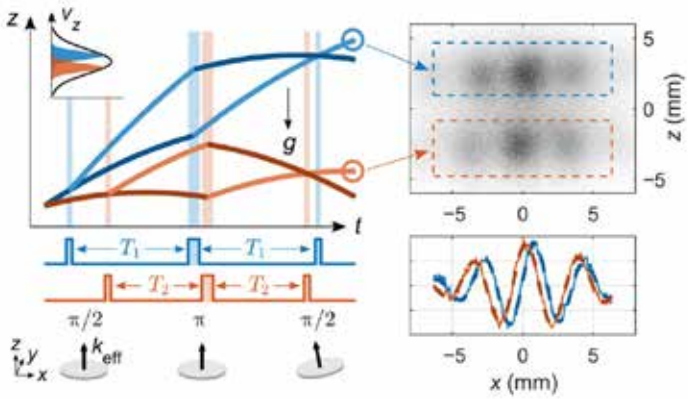

FIG. 1: Two atom interferometers are simultaneously operated on the same atomic ensemble, allowing to extract two phase measurements which together uniquely determine the inertial phase over a much larger dynamic range.

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Effects of deuteration on the reaction dynamics of F^- with CH_3I.

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Our group studies ion-molecule reactions using a crossed-beam setup with kinematically complete velocity map imaging (VMI). This has proven to be a powerful tool to obtain experimental insight into molecular reaction dynamics, as the obtained differential cross sections can be used to link and identify atomistic reaction mechanisms during the formation of reaction products. In recent experiments we have investigated the reactive scattering of fully deuterated methyl iodide CD_3I with atomic fluorine anions in the energy range from 0.7 to 2.3 eV relative collision energy. The results are compared with the hydrogenated system F^- + CH_3I [1] as well as quasi-classical trajectory (QCT) simulations [2]. The two main reaction channels are nucleophilic substitution (S_N2) and deuteron/proton transfer for both systems. The F^- + CH_3I reaction shows a significant large-impact parameter contribution in the S_N2 channel, a feature that is absent for its deuterated counterpart. While the simulations can fully capture the S_N2 dynamics in the reaction with CD_3I, large-impact parameter events from F^- + CH_3I cannot be reproduced. Such a discrepancy between experimental and theoretical work might hint towards a quantum effect that cannot be captured by QCT simulations.

We also present preliminary results on the reactive scattering of CH_3I with radical anions, more specifically with atomic oxygen anions O^-. We discuss energy-dependent differential cross sections and branching ratios for four observed, competing reaction pathways.

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Reflection and Refraction of a Photon using a New Mathematical Photon Model

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There is growing interest to study a single photon generation, detection and its properties, because the single photon is considered as the main element in quantum communication, where it is important to know how the single photon is reflected, refracted and diffracted. But there is not a complete understanding of what a photon is exactly. The quantized field with the creation and annihilation operators is not suitable to describe these processes.

We propose a new three-dimensional photon model [1,2], where the free propagating photons are described by the vector potential, satisfying three independent linear equations for three coordinates – for the longitude coordinate it is the equation of harmonic oscillator and for the transverse coordinates they are equations with the solutions of the Gaussian functions. The interaction potential between the photons and the charged particle differs from the potential derived by the traditional quantization method only with the definition of the harmonic oscillator coordinates.

To validate the model for a photon reflection and refraction of photons on the boundary between two dielectrics is considered [2]. The amplitude of the reflected photons is determined by the Fresnel formula, such as for the plane waves, but the amplitude of the transmitted photons is different. The transverse size of the transmitted photons in the plane of incidence changes with the angle of incidence changing (see Figures 1 and 2).

The main conclusions of this research are:

1) In our model the transverse size of transmitted photon changes, that could be possible observed experimentally (see Figure 1).
2) For both components (parallel, as well as perpendicular) the following relation for the amplitudes of incident, *I*, reflected, *R*, and transmitted, *T*, fields fulfil: $R^2/I^2+T^2/I^2=1$. Both terms can be interpreted as the probabilities for a photon to be reflected or transmitted similarly as in quantum mechanics. Classically, part of the field is reflected, and the other part is transmitted.

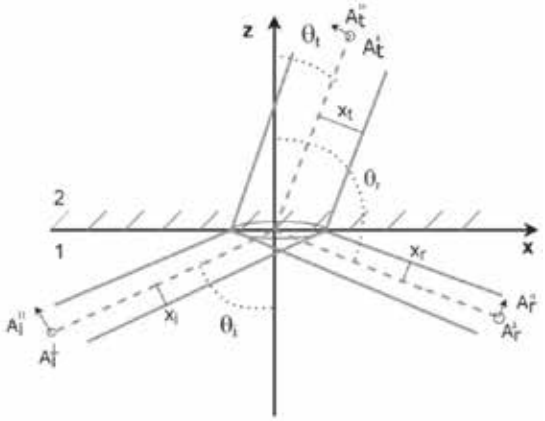

FIG. 1: Reflection and refraction of photons. Plane of incidence.

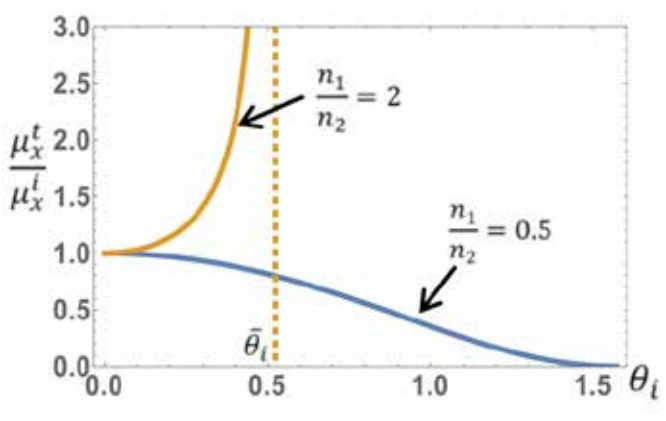

FIG. 2: The ratio of parameters for the transmitted and incident photons as a function of the angle of incidence. n_i are the refractive indexes and θ_i is the critical angle of total reflection.

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Theoretical study of TPPS4 monomers and dimers including their spectra

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In the past few decades, 5,10,15,20-tetrakis(4-sulfonatophenyl) porphyrin (TPPS4) molecules have been extensively investigated because they efficiently self-associate from monomers to large H- or J- aggregates in aqueous media depending on the pH value and on compound concentration. It is still not understood what type of aggregates are formed in specific conditions. To address this question we study how small dimeric structures are formed and how these primary aggregates can be observed in absorption and electronic circular dichroism (ECD) spectra.
The goal of this study is to determine the most stable TPPS4 dimers and simulate their absorption and ECD spectra. To achieve this goal, we aim to determine the most stable $H_4TPPS_4^{2-}$, $H_6TPPS_4^{0}$ and $H_8TPPS_4^{2+}$ monomers structures, investigate their all possible H- and J-dimer configurations and model spectra.
The structures of TPPS4 monomers were determined using DFT B3LYP with the Pople 6-311G(d,p) basis set, while the structures of dimers- with CAM-B3LYP/6-31G(d,p) method. The spectra were calculated with TD-DFT B3LYP/6-31G(d,p) method. PCM was used to evaluate the influence of water. In this research, the Gaussian 16 C.01 [1] and GaussView 6.1 [2] programs were used.
Four different monomers were selected and 9 dimers (as in example see Fig.1) were constructed. It was established that different structures are characterized by different absorption spectra. Moreover, different structures yield different chirality and the corresponding ECD spectra due to distinct protonisation patterns.

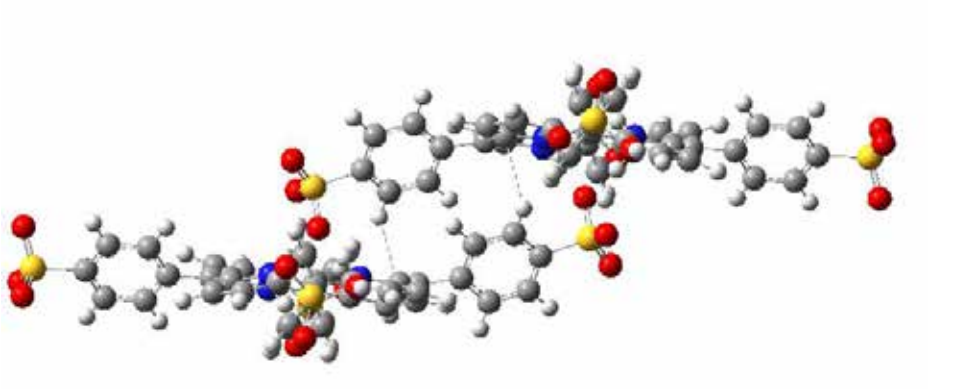

FIG.1: $TPPS_4$ dimer.

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Mechanism of surface nanostructures formation in the interaction of slow, highly charged xenon ions with the gold nanolayers

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Research on the design and manufacture of new materials with unique physical and chemical properties, in particular materials using nanometer size structures, are fundamental to the development of many areas of science. Due to the exhausting potential of currently used technologies, extensive research is carried out around the world to better understand the mechanisms of surface nanostructures formation and to develop a new, repeatable and effective methods for their production.

In this work we have systematically studied process of energy deposition and formation of nanostructures on metallic (Au nanolayer) surfaces as a result of the irradiation with single low-energy highly charged xenon ions (HCI). The irradiations were performed at the Kielce EBIS facility (Jan Kochanowski University, Kielce, Poland) for constant kinetic energy 280 keV and different charge states (Xe^{q+}, q = 25, 30, 35, 36 and 40), and for constant charge state Xe^{35+} and different kinetic energies: 280 keV, 360 keV, 420 keV and 480 keV of the HCI. This allowed for the independent study of the influence of kinetic energy and neutralization energies of the HCI on the shape of the produced nanostructures produced on Au nanolayers [1, 2].

The results are interpreted within recently developed micro-staircase model based on the quantum two-state vector model of the ionic Rydberg states population [3]. In this model the formation of the nanostructure is governed by the processes of the ionic neutralization in front of the surface and the kinetic energy loss inside the solid. The interplay of these two energies in the surface structure creation is described by critical velocity. Using the model neutralization energy, deposited kinetic energy and critical velocities were calculated and compared with experimental results.

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Total Reflection X-ray Photoelectron Spectroscopy in Analysis of Ti and TiO_2 Surfaces

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X-ray photoelectron spectroscopy (XPS) is well known technique of surface analysis [1], in which a low energy X-ray beam (for example Al-Kα) is directed towards the studied surface at an angle of several tens of degrees resulting in emission of electrons from the surface, which are next analyzed by an electron analyzer. The sensitivity of this technique can be improved by applying the phenomenon of total reflection of X-ray radiation when the excitation beam is directed at the analyzed sample at an angle smaller than the critical angle [2, 3]. The value of this angle depends on the radiation energy and the sample material. Such modified technique is known as the total reflection X-ray photoelectron spectroscopy (TRXPS) [3, 4]. Under total reflection condition, the X-rays cannot penetrate the surface deeper than the evanescent length, usually 20–40 Å. The intensity of X-rays in the evanescent range can be as much as four times stronger than the intensity of the primary X-ray beam because of the standing-wave formation on the surface. Consequently, the photoelectron signal of atoms in the surface region is increased. Application of such geometrical condition results in the reduction of background in XPS spectra, to less than half of that for the normal incidence X-ray photoelectron spectra, also due to the lower inelastic electron scattering. Therefore, background reduction is the most essential effect of total reflection conditions [3].

In presented study, TRXPS method was applied in analysis of Ti and TiO_2 surfaces deposited on Si and SiO_2 substrates, before and after surface modification with slow highly charged Xe^{q+} ions. The aim of the study was to determine the changes in chemical-physical properties of nanolayers as results of ions-surface interaction. The samples were modified with slow Xe^{q+} ions delivered by EBIS accelerator at the Institute of Physics of Jan Kochanowski University (JKU) in Kielce (Poland) [5]. The TRXPS measurements were carried out using XPS system (SPECS). For comparison also XPS measurements, in non-total regime, were performed.

In the TRXPS and XPS measurements both survey and detailed spectra (photoelectron peaks C1s, N1s, Ti2p and O1s) were investigated. The measurements gave information about the surface properties of Ti and TiO_2 nanolayers (electron binding energy, elemental composition, chemical environment of the elements). It was shown, that the use of TRXPS geometry increases the intensity of the photoelectron lines and at the same time lowers the background in XPS spectra. The structure of the C1s, N1s, Ti2p and O1s photoelectron peaks were discussed in details and compared for surfaces before and after modification with slow highly charged Xe^{q+} ions.

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High Efficiency Continuously Tunable Subnanosecond Optical Parametric Generator-Amplifier Based on MgO:PPLN Crystal

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A simple single-pass setup of the optical parametric light generators (OPGs) enables to obtain compact, continuously tunable laser radiation sources that are less costly and more resistant to external disturbances compared to optical parametric oscillators. Subnanosecond (100 ps – 1 ns) OPGs are needed for applications where high temporal resolution supplied by expensive ultrashort (<10 ps) laser systems is redundant, but nanosecond (>1 ns) temporal resolution is insufficient. Applications are spectroscopy, gas detection, microscopy, biological studies, and THz generation to name a few, but even in the case of high demand for such devices, subnanosecond pulse duration OPGs are not widely developed [1,2]. However, advances in micro-laser manufacturing technologies allows them to be used as a high energy pump source for OPGs and coupled with very high nonlinearity periodically-poled crystals as a gain media, efficient subnanosecond parametric generators could be developed. Detailed theoretical and experimental investigation of such OPGs is necessary in order to create a commercially attractive product.

Here we thoroughly investigate 2 cm long MgO doped periodically-poled lithium niobate (MgO:PPLN) crystal based OPG pumped by subnanosecond pulses from a passively Q-switched Nd:YAG micro-laser. Continuous tuning of signal wave wavelength in 1442 - 4040 nm spectral range was achieved by varying the grating period and the temperature of the crystal, whereas total OPG conversion efficiency reached (record high) up to 46% and depended on the grating period (Fig. 1). Experimentally measured spatial, temporal and spectral characteristics of the generated light are presented and supplemented by the numerical simulations based on the quantum mechanical model. By injection seeding the OPG with narrowband CW laser source, signal wave generation threshold was reduced, and efficiency was increased while simultaneously obtaining very high spectral power density output pulses.

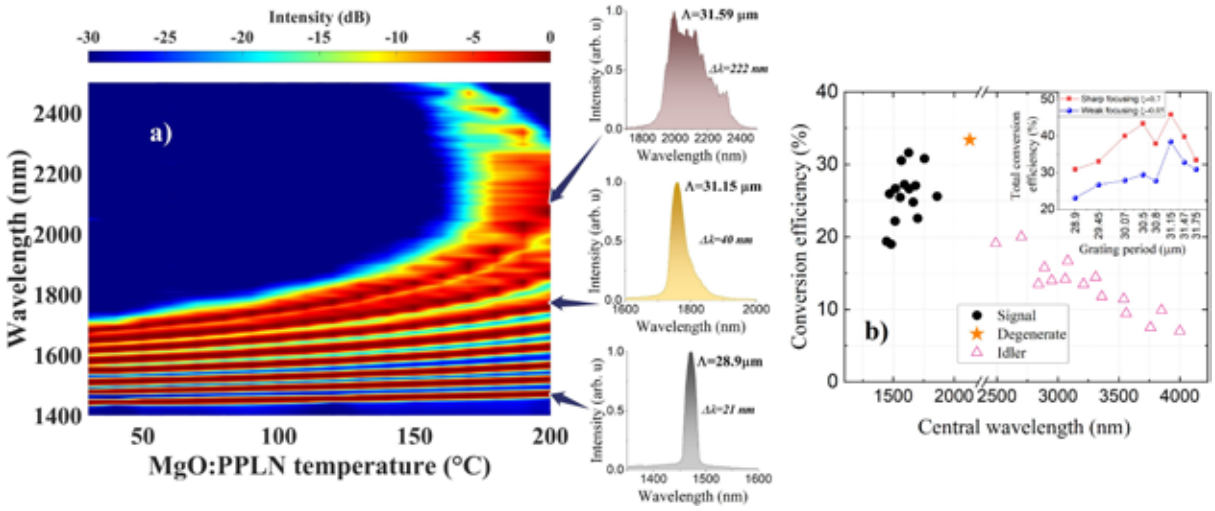

FIG. 1: Signal pulse spectral envelope evolution with varying MgO:PPLN crystal temperature for 8 gratings (a). (b) – OPG conversion efficiency distribution at different OPG wavelengths.

This work has received funding from European Regional Development Fund (project No. 01.2.2-LMT-K-718-03-0004) under grant agreement with the Research Council of Lithuania (LMTLT).

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Non-homogeneously polarized optical Airy-like beams

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Laser beam shaping has found applications and uses in many different areas of research and industry, including telecommunications, optical particle manipulation, microscopy [1] and many others. With current technology, it is possible to precisely modify the parameters of light, such as phase, polarization, and amplitude. The use of various meta-materials, spatial light modulators, geometrical phase elements and other tools and methods made it easier than ever to put ones theories into experiments.

One intriguing family of electromagnetic beams that is well studied is so-called non-diffracting optical beams. This means that they have a longer diffraction-free region than known Gaussian-type beams. Examples of such beams include Bessel beam, Airy beam [2], Mathieu beam, and others. Airy beams excel in a few different situations compared to other non-diffracting beams. Firstly, they are shown to be robust, which means that they can regenerate their profile after propagation in a turbulent environment. Secondly, because of its curved intensity distribution Airy beams can accelerate small particles in a curved trajectory and be used for particle clearing.

In this work, we investigate Airy-like optical beams with a non-homogeneous polarization distribution. Mostly scalar versions of beams are studied extensively, and vector qualities of the beams are neglected. By using standard method introduced by Morse and Feshbach [3], one can construct electric and magnetic vector fields from a scalar field representing wave solution. This method is used to obtain Airy-like vector beams. Firstly, two vector solutions representing magnetic or electric vector fields are obtained. Secondly, for experimental purposes, a Fourier spectrum for both vector beams is calculated. Both the intensity of the vector field and the spectra of the field components are discussed and analyzed.

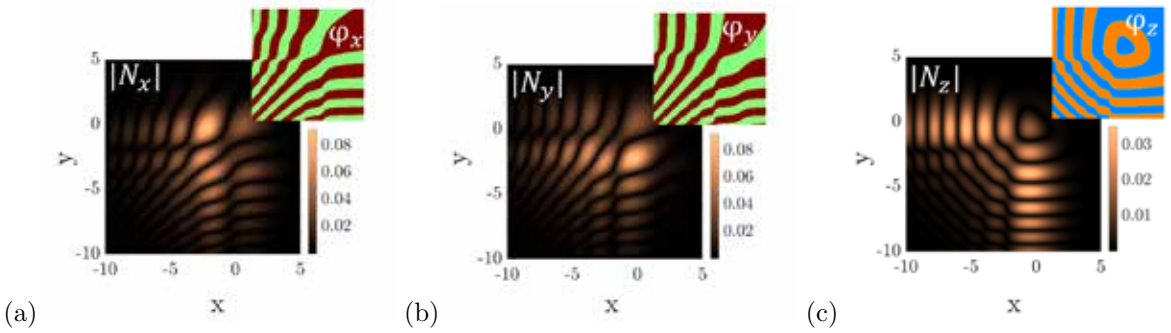

FIG. 1: (a-c) Absolute value of the amplitude distribution for the electric type Airy-like vector beam at $z = 0$ for components N_x, N_y and N_z. Amplitudes are normalized to the maximal value of the beam and the inserts show the phase for each component of the field. The wavenumber $k = 2\pi$

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Radio Frequency Atomic Magnetometers for Non-Destructive Inductive Measurements

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In recent years, atomic sensors have gained significant interest due to their outstanding performance. Atomic magnetometers can achieve state-of-the-art sensitivities with a favourable size, weight, and power [1]. The overall simple sensor architecture, requiring only a few elements, makes them attractive for miniaturisation and are already commercially available [2, 3]. These sensors can be configured to measure rf magnetic fields, which opens a wide range of application areas from biological imaging [4], under-water/ -ground communication [5], and non-destructive testing (object/defect detection) through inductive measurements [6-8]. Our group at NPL has built an unshielded magnetometer, Fig. 1 (a), than can operate in a noisy laboratory and achieve a sensitivity of ~50fT/sqrt(Hz) [9].

Inductive measurements are a widely deployed tool for non-destructive testing, where an rf field called the primary field couples to an object through its electric conductivity or magnetic permeability, and the object generates an rf field in response called the secondary field. Mapping how the secondary field changes across the object can reveal specific properties, such as material composition, shape, orientation, and structural inhomogeneities. We referred to this technique as magnetic induction tomography (MIT), although it has several other names (commonly eddy current testing). The advantage of MIT is that rf fields can propagate through solid objects, layers of different material and free-space, unlike ultrasound testing or infrared imaging. Pick-up coils have been used for this application; however, their sensitivity decreases at low frequencies, where penetration depth is greatest. The rf magnetometer is highly attractive because of its superior sensitivity at low frequencies for a sensing area of the same size.

The author will discuss the unique functionalities of the rf magnetometer that can be exploited to improve MIT, such as vectorial field measurement, an insensitive axis that can remove the dominating primary field from the measurement, and an active mode of operation which increases sensor bandwidth. These features can be configured to carry out high contrast and resolution defect detection [Fig. 2 (a)], identify material composition [Fig. 1 (c)], increase measurement speed.

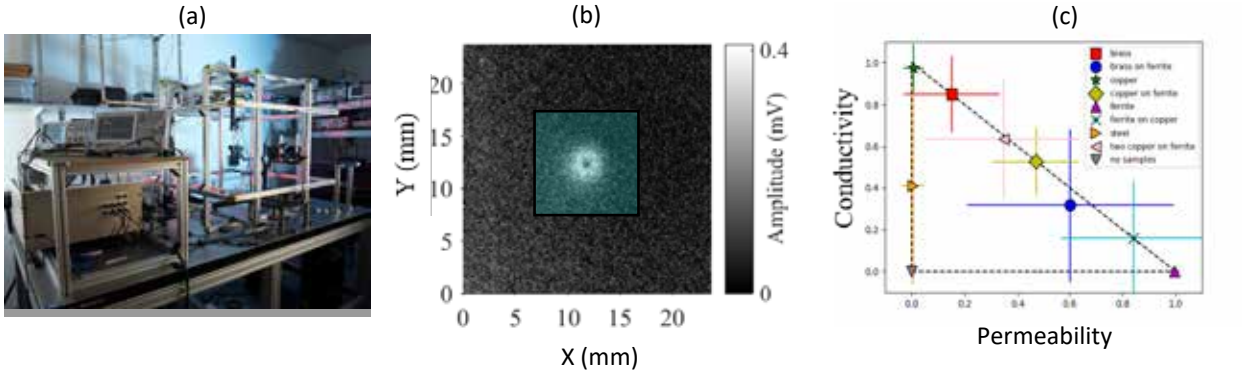

Figure 1. (a) Photograph of lab based setup containing lasers and controllers, magnetitic field coils, sample translation stage, and detection optics. (b) Image recorded for a 1 mm diameter recess (mimicking a defect) recorded with a 1 cm3 rf atomic magnetometer (outlined by faint blue rectangle) positioned 30 cm along the Z-axis from the sample. (c) Machine learning is used to discriminate between different materials by assigning parameters to the data recorded for each sample.

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S1-P19

Towards Quantum Control of Calcium Ions for the use in Molecular Spectroscopy

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We present our advances towards establishing a new two dimensional spectroscopy method that selectively identifies the suitable quantum states. For this purpose, the molecular ions to be investigated are sympathetically cooled and trapped in an ion trap with laser-cooled calcium ions [1]. We will use the photon-recoil spectroscopy method to study the molecular ions through studying the photon-recoil imparted on co-trapped calcium ion [2].

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Optical diagnostics in cold plasmas and atomic spectroscopy

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Optical diagnostics, in cold plasmas, is, to a great extent, based on two-photon absorption laser induced fluorescence (TALIF). The non-linear character of the excitation scheme can make the technique spatially selective, with a detection signal at a wavelength different from that of the excitation laser, hence more easily filtered out.

In typical TALIF experiments, however, the quantity under scrutiny is the density or (inclusively) the temperature of some atomic species. Measurement of the former quantity can only be achieved provided that the excitation and detection efficiencies have been calibrated. As far as atomic oxygen density measurement is concerned, part of the difficulty can be circumvented by comparing the fluorescence output with the fluorescence obtained from atomic xenon, the density of which can be easily known, thanks to a very similar excitation and fluorescence scheme. However, oxygen and xenon have different two-photon excitation cross-sections, which must both be known, or the ratio of which must have been calibrated too.

Scarcity of the available data led us to directly measure two-photon absorption in a 0.5 m long xenon cell, in order to get an original measurement of the generalized cross-section. The integrated cross-section was found equal to $1{,}36^{+0{,}46}_{-0{,}34} \times 10^{-43}$ m^4 and $1{,}88^{+0{,}75}_{-0{,}54} \times 10^{-43}$ m^4 for the 6p'[3/2]$_2$ and 6p'[1/2]$_0$ levels of xenon, respectively. In the first case, this is twice smaller than the value found hitherto in the literature, which was $3{,}6^{+1{,}7}_{-1{,}4} \times 10^{-43}$ m^4. As a consequence, atomic oxygen densities formerly deduced from a calibration on the 6p'[3/2]$_2$ level of xenon must be divided by a factor of 2, in retrospect [1].

Alternatively, temperature measurements that rely on the measurement of Doppler broadening must take into account the underlying hyperfine structure. Hyperfine parameters A and B of the singly-excited levels of xenon show a great variety, which can be however completely explained by the hypothesis that most of the hyperfine interaction is that of the p^5 electron core with the nucleus, with a dependence on the angular quantum numbers that just reflects the way the core angular momentum j_C gets projected on the total electron angular momentum J (figure 1) [2]. Explicit formulae will be given at the conference.

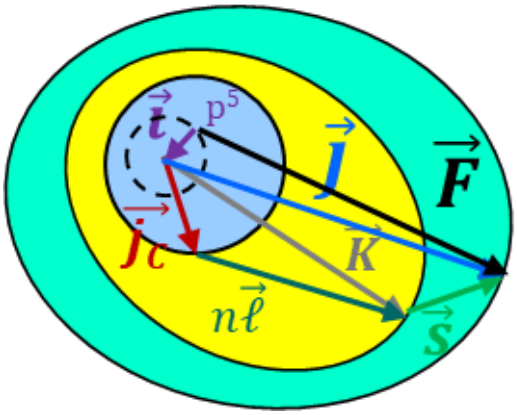

FIG. 1: The internal angular momenta of xenon, in the so-called Racah coupling scheme. Based on that scheme, angular momentum algebra makes it possible to outline the variations of the hyperfine parameters.

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Ultra-cold potassium-cesium mixtures in an optical dipole trap

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We present our recent results on the production of ultracold mixtures of ^{39}K+Cs and ^{41}K+Cs confined in an optical dipole trap. We obtain samples of nearly $5{\cdot}10^5$ atoms of each species at ∼10 µK which is a good starting point for studies of collisional properties of the ^{39}K,^{41}K+Cs mixture (in particular, search for Feshbach resonances) as well as for photoassociation spectroscopy required for the formation of ground state molecules.

We begin by simultaneous trapping of cesium and one of the potassium isotopes in magneto-optical traps, while minimizing losses due to heteronuclear collisions. After the compression of the clouds by increasing the magnetic field gradient and appropriately red-detuning trapping beams, we apply gray molasses cooling techniques to both species. The potassium isotopes are cooled to ∼10 µK using gray molasses on the D1 line, while for cesium we use light near the D2 line. The dipole trap loading immediately follows the sub-Doppler cooling stage. Our studies have shown that the experimental sequence optimized for loading the dipole trap with only a single species needs to be only slightly modified for the mixture and requires minor timing changes to match the cooling steps for cesium and potassium.

The mixture is trapped in a single-chamber system, where dispensers placed at a distance of about 10 cm from the center of the optical dipole trap are the only source of atoms. By proper balancing the current running through the dispensers and the light-induced atomic desorption timing we obtain single species lifetime exceeding 10 s, sufficient for most applications, possibly even including reaching simultaneous quantum degeneracy.

In future experiments, we will pursue the search for Feshbach resonances in the ^{41}K+Cs mixture and photoassociation spectroscopy of KCs to identify a suitable pathway for reaching the ground state of the molecules with STIRAP [1, 2].

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S1-P22

The accelerator on a chip: Progress and potential biomedical applications

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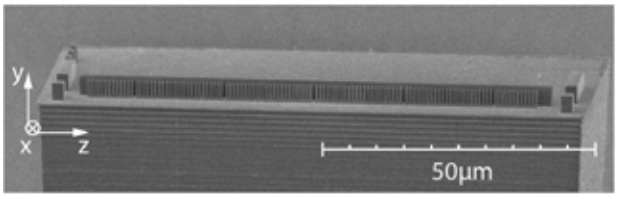
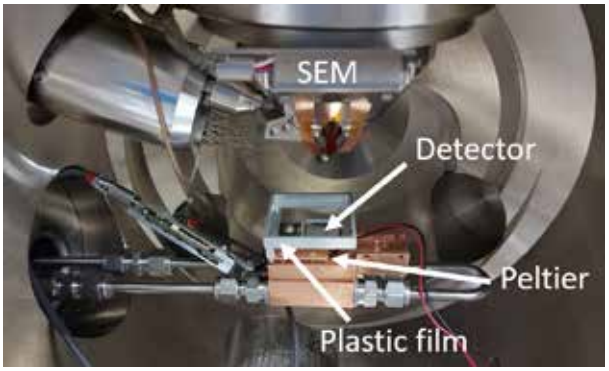
Dielectric laser accelerators (DLA) are a highly promising technology that enables the miniaturiziation of conventional particle accelerators to tabletop or even microchip size. A DLA consists of a silicon nanostructure (Figure a) that is illuminated with a pulsed laser beam. This creates an evanescent near-field that can accelerate electron pulses entering the structure. To reach high energies with this scheme, it is necessary to extend this interaction from the previous tens of micrometers length scale to millimeters or more. This is challenging as the electrons also experience transverse deflecting forces in the nanostructure and are eventually lost. To counteract this, we have employed an alternating phase focusing scheme. By building phase jumps into the structure, the electrons are subjected to alternating transversal focusing and defocusing forces, effectively guiding the beam through the structure. We have demonstrated successful guiding of a 28.4 keV electron beam through the narrow, 225 nm wide channel of a 77 μm long nanostructure [1].

One of the most important applications of accelerators is in biomedical research and radiation therapy. A miniaturized accelerator might not only reduce the cost of such machines, but also lead to new therapy modalities such as an endoscopic device that can irradiate tumors from within the body, reducing the damage to unaffected tissue. To begin exploring the potential for biomedical applications, we are preparing an experiment for a dosimetric characterization of a DLA. Since the beam energy is as of now lower than conventional linear accelerators, typical dosimetry methods can not be used. To work towards dosimetry of such low-energy beams, an electron beam from a scanning electron microscope (SEM) is used as a reference. A Timepix particle detector is used to detect electrons and measure their energy spectrum. (Figure b) Expected dose distributions are simulated with the package Geant4. The simulations are compared with transmission measurements on plastic film samples. These measurements will soon be extended to use biological samples.
In this contribution, we will give a status update on the experimental progress towards advanced nanophotonics-based electron beam control and the dosimetry of such beams.
We gratefully acknowledge funding from the Moore Foundation (ACHIP) and ERC (AccelOnChip).



(a) SEM image of a DLA structure. Electrons pass through the channel in z-direction. The laser is incident from the x-direction and is reflected by Bragg mirrors behind the channel, creating a symmetric field in the structure.



(b) The setup for dosimetry of low-energy electrons. A temperature-stabilized Timepix particle detector measures the energy spectrum of electrons from a SEM. Plastic films of varying thickness are placed in between to simulate transmission through thin water layers.

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Nonlinear exciton equations at fifth order to the optical field: Intensity dependent nonlinear spectra dynamics in J-type aggregate

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Specific dye molecules can self assemble into aggregates in variety of configurations[1]. Electronic optical excitaton of such systems results in the large exciton formation. I. e. the molecular excitations tend to be shared by the dye molecules in quasi Bloch wave-like exciton fashion.

Such character of wavefunctions create a fundamental theoretical challenge when modeling such systems because of incompatibility of local and delocalized properties. Note that molecular vibrations, which is the source of exciton decoherence and thermalization, are local characteristics of dye molecules. More complex exciton decay channel - excitation annihilation, is also the local property. Combining local and delocalized properties becomes the limiting factor in developing efficient theory for describing such systems. We have developed nonlinear exciton equations(NEE) with terms up to fifth order to the optical field to account for exciton exciton annihilation process[2].

Double walled tubular J aggregate systems are composed of huge amount of molecules and the calculation of full exciton dynamics is unfeasible. It has been suggested that the two lowest bands form independent uncoupled domains with J band type characteristics[3]. We thus suggest that for such type of systems the spectroscopy features of the two lowest absorption peaks can be described as of two independent superradiant J-type features that can be modeled as separate J aggregates.

We suggest that nonlinear properties of such systems can be efficiently approximated by including only several excitons thus restricting exciton band to its properties around band minimum. For experimental observations we employ nonlinear exciton equations with exciton-exciton annihilation terms.

We calculate excitation intensity dependent pump-probe spectra (Figure 1) and show that exciton population decay dynamics are faster at higher excitation intensity. This result was acquired using reduced system of 15 excitons from 200 sites.

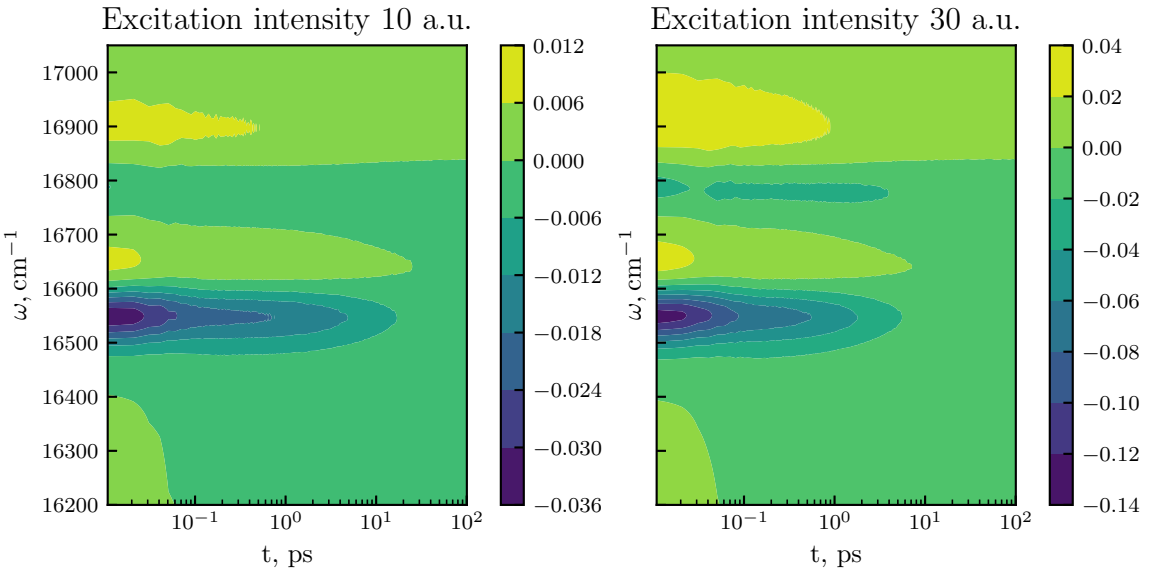

FIG. 1: Calculated pump probe spectra dependence on delay time t, and pump pulse intensity.

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Subwavelength Raman lattices with time-dependent detuning

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Ultra-cold atoms in optical lattices have demonstrated utility for simulating various condensed matter phenomena as well as realizing paradigmatic models. However, conventional optical lattices for ultra-cold atoms rely on the AC Stark shift to produce a potential proportional to the local optical intensity. As a direct result, the lattice period cannot be smaller than half the optical wavelength λ. Recently, two techniques have emerged to create deeply sub-wavelength lattices [1, 2, 3]; both can be understood in terms of "dressed states" created by coupling internal atomic states with one- or two- photon optical fields.

Here we focus on the scheme depicted in Fig. 1(a), relying on sequentially coupling N internal atomic states using two photon Raman transitions [1]. This results in an adiabatic potential for each of the N dressed states, displaced by $\lambda/2N$ from each other as shown by the dashed curves in Fig. 1(b). We show that adding temporal modulation to the detuning from Raman resonance can couple the s and p bands of adjacent lattice sites belonging to different dressed states. In the tight-binding limit, this gives rise to a pair of coupled Rice-Mele (RM) chains with new regimes of topological charge pumping. The present study opens new possibilities in studying the topological properties of subwavelength optical lattices induced by periodic driving.

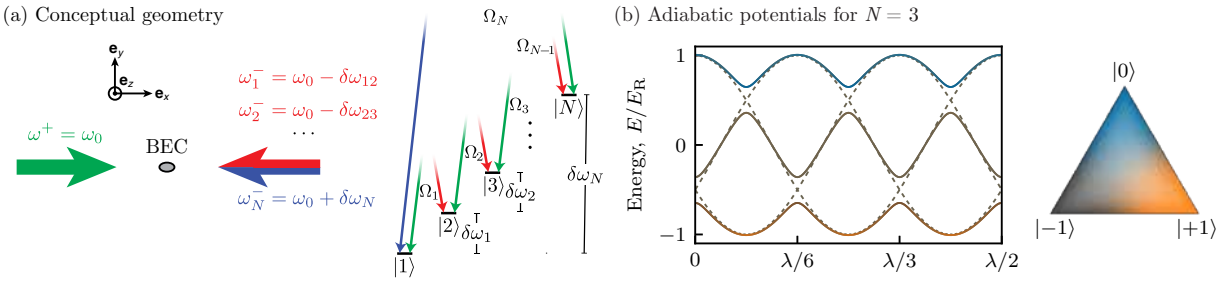

Figure 1: Lattice concept. (a) Representative experimental geometry with a single frequency Raman beam traveling along $\mathbf{e}_x$ and N beams sharing the same spatial mode traveling along $-\mathbf{e}_x$. The level diagram for cyclic coupling is depicted on the right. (b) Dressed state energies for $N = 3$. The dashed curves are computed for $\Omega_1 = \Omega_2 = \Omega_3 = E_{\text{recoil}}$ and the colored curves are computed with a non-zero detuning.

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Atomic Clock Ensemble in Space

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The Atomic Clock Ensemble in Space (ACES) mission is developing high performance clocks and links for space to test Einstein's theory of general relativity. From the International Space Station (ISS), the ACES payload will distribute a clock signal with fractional frequency instability and inaccuracy of 1×10^{-16} establishing a worldwide network to compare clocks in space and on ground. ACES will provide an absolute measurement of Einstein's gravitational redshift, it will search for time variations of fundamental constants, and perform Standard Model Extension tests.

The flight models of the ACES instruments and subsystems are under completion. System tests involving the laser-cooled Cs clock PHARAO, the active H-maser SHM and the on-board frequency comparator (FCDP) have measured the performance of the clock signal delivered by ACES. The ACES microwave link MWL is currently under test. The single-photon avalanche detector of the ACES optical link ELT has been tested and it is now waiting to be integrated in the ACES payload.

The ACES mission concept, its scientific objectives, and the recent test results will be presented together with the major milestones that will lead us to the ACES launch.

FIG. 1: Flight model of the ACES payload before system tests.

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Stochastic methodology for superradiance based on positive P representation

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As highlight in [1], "... the problem of superradiance in free space is in general a problem of three-dimensional non-linear diffraction theory, further complicated by the quantum nature of the radiated field at the early stage of the emission process..." Due to the acknowledged complexity of the problem, the theoretical work within this field is typically focused on a specific aspect of this collective emission phenomenon. Our goal is to develop a general formalism grounded on rigorous derivations and suitable for characterization of superradiance in distributed systems of atoms experiencing various incoherent processes such as dephasing, pumping, Auger decay. The novel framework builds a solid foundation for future, quantitatively predictive investigations of light-matter interaction in realistic conditions.

The formalism is based on the generalized positive P representation for bosons. To introduce atoms into the formalism, we bosonize them with Jordan-Schwinger transformation. The resulting equations are convenient for numerical analysis and possess an intuitive structure. For instance, light-matter interaction with all subtle quantum effects requires equations similar to the Maxwell-Bloch ones. The only difference is that they include noise terms as a source. In the case of superradiance, these noise terms can be interpreted as the initial spontaneous emission triggering the process.

Practically, numerical implementation is quite sophisticated and requires stochastic gauging [3]. To demonstrate the formalism in operation, we present the detailed description of superradiance in compact systems. Besides, we demonstrate some numerical results for realistic distributed systems.

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S1-P27

Photoionization of Polarized Xe Atoms in a Magnetic Field

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Ionization of two-photon excited states $5p^5(^2P_{3/2})6p[3/2,5/2]_2$, $M = 2$ (jl-coupling) of xenon atoms by circularly polarized probe light was studied experimentally in a supersonic beam. The observed photoionization signals revealed oscillation structure due to the Larmor precession of atomic states in an external magnetic field. We derived analytical formulas for the photoelectron current and explained the diversity in the structure of the detected oscillations in terms of the principal lines among multiplet components of optical transitions. The obtained numerical data demonstrate collapse and revival (beating) behavior of the photocurrent due to nonlinearity of Zeeman shifts in the presence of the Paschen–Back effect. Our results indicate the possibility of implementing Doppler-free spectroscopy involving bound-free transitions.

This work is supported by the Latvian Council of Science project No. LZP-2019/1-0280.

Optimal Adiabatic Passage Parameters for Tripod Quantum Systems

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Stimulated Raman adiabatic passage (STIRAP) [1] is a robust method for selective population transfer between quantum states with multitude of applications in contemporary physics, chemistry and information processing. STIRAP in tripod systems [2] is particularly interesting to quantum information because of the two (degenerate) dark states. This set of dark states can form a qubit, and several methods for implementing quantum gates in N-pod systems have been proposed. Our present research focuses on exploring the optimal pulse sequences for tripod STIRAP.

We demonstrate how a purely geometrical interpretation of tripod STIRAP can be used to determine the optimal laser pulse sequence. The bright state $|Br\rangle \propto \Omega_P |1\rangle + \Omega_Q |4\rangle + \Omega_S |3\rangle$ is associated with a unit vector $\overrightarrow{R}$ in a three-dimensional parametric space of laser Rabi frequencies Ω_i. The two degenerate dark states $|D\rangle = a_P |1\rangle + a_Q |4\rangle + a_S |3\rangle$ lie in the two-dimensional tangent space to the unit sphere at point $\overrightarrow{R}$. Temporal evolution of the Rabi frequencies describes a path $\overrightarrow{R}(t)$ on the surface of a unit sphere, and temporal evolution of the dark states is a direct consequence of Riemannian parallel transport of the "dark" tangent space along this path. Combining this approach with the optimal adiabaticity condition for resonant STIRAP $\sum_i \Omega_i^2 = \text{const.}$, we obtain the optimal pulse sequences for high-fidelity tripod STIRAP (FIG. 1), including fractional STIRAP. In contrast to the conventional STIRAP in Λ system, the optimal laser pulses can be approximated with realistic Gaussian laser pulses without significant detrimental effects [3] to transfer fidelity.

This work is supported by the Latvian Council of Science project No. LZP-2019/1-0280.

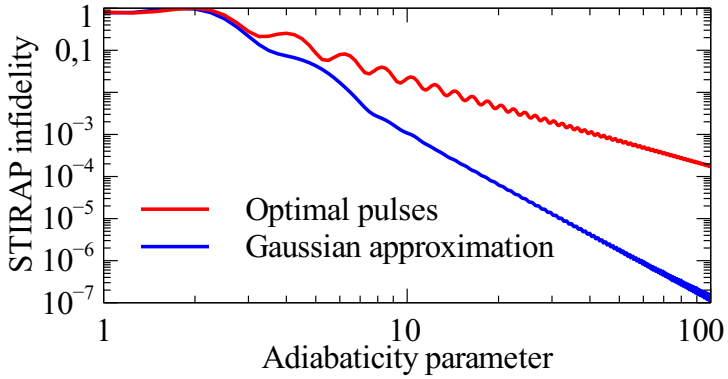

FIG. 1: Infidelities of full STIRAP in tripod system for both optimal pulse sequence and its approximation with Gaussian pulses follow a power law relationship.

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Three-Dimensional Single-Shot Coherent Diffraction Imaging of Silver Nanocrystals

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Coherent Diffraction Imaging (CDI) is a lens-less technique that aims at retrieving spatial information of an isolated sample from the scattering amplitude of a highly coherent and monochromatic light beam [1]. Thanks to the ultra-short, high-intensity and high-energy light pulses provided by Free Electron Lasers, CDI allows snapshots and time-resolved "movies" of isolated samples down to the nanoscale. The lack of optical devices makes CDI an indirect imaging method, and sophisticated numerical analyses are required to retrieve the sample image. In the small-angle scattering regime, the diffraction pattern is proportional to the squared amplitude of the Fourier Transform of the sample's 2D projection along the beam direction, which can be effectively reconstructed by the use of phase retrieval algorithms [2]. On the other hand, in the wide-angle scattering regime, a single diffraction pattern carries 3D structural information on the sample [3]. However, the non-trivial mathematical link between the sample's 3D shape and the diffraction pattern renders 3D single-shot CDI a scientific challenge. Here we present a 3D reconstruction method from single-shot wide-angle diffraction patterns based on a classical *forward-fitting* procedure, which is founded onto three main pillars: (i) a fast simulation method [4] based on Multi-Slice Fourier Transform (MSFT), (ii) a sufficiently generic parametrization of the sample's shape, and (iii) a wise optimization strategy. Three-dimensional reconstructions are performed from wide-angle diffraction images acquired at the CAMP endstation at the soft X-Ray Free-Electron Laser FLASH in Hamburg. There, individual unsupported silver nanocrystals of 70nm average size were characterized with CDI using a wavelength of 5.1nm. For the imaging procedure, the sample is parametrized as a convex 3D polygon with uniform refractive index, without any additional constrained symmetry. Three-dimensional reconstructions show satisfactory reliability and consistency, with an almost complete independence upon the starting guess of the optimization procedure. The retrieved shapes of the silver clusters agree in many cases perfectly with results from a previous work [3], correctly reproducing the expected crystalline symmetries. In addition, two new structural motives were identified, tetrahedral shapes and trigonal platelets (see Figure 1), which testify for the dependence of the surviving seed structure on the exact experimental conditions in an early stage of their formation. The imaging method is then further extended to nanocrystals agglomerates, allowing for the first time a direct insight into their growth process. The relevance of the presented results goes well beyond this specific dataset. Indeed, this work represents a strong proof of concept for this imaging approach, raising the bar of the capabilities of 3D coherent diffraction imaging from single shot.

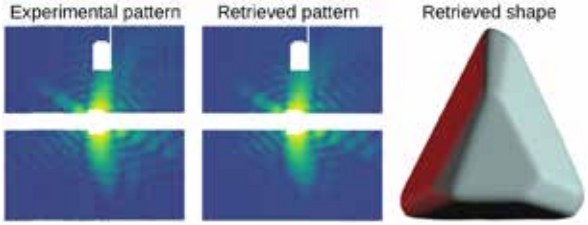

Figure 1. Reconstruction example of a faceted silver cluster with truncated tetrahedral shape, imaged with 5nm radiation wavelength.

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Robustness analysis of a modified quantum random walk search algorithm

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Quantum random walk search [1], together with the Grover's search [2], are quantum algorithms for search in an unordered database. However, unlike Grover's one, random walk search can be used with arbitrary topology. The fundamental building blocks of this algorithm are: Walk and Mark coins, Shift operator and Oracle. Both Oracle and Shift operators cannot be modified for chosen topology and number of solutions. In this case quantum algorithm could be improved by modifying the walk-coin. Coins build by Householder reflection are already used to study and optimize the algorithm. For example, the impact of systematic phase errors in quantum walk search operators on its success rate, has been studied in [3] through theoretical analysis and numerical simulations.

Our previous work [4] elaborates on modification of the quantum random walk on hypercube. This algorithm has high robustness to deviations in the walk-coin's parameters, namely Householder reflection phase and a newly introduced phase factor. Monte Carlo simulations, in combination with supervised machine learning, were used to find relations between these phases, and so drastically increasing the stability of future implementations of quantum walk search algorithm where the systematic deviations in the quantum computer's physical parameters could not be ignored.

Here, we present the results of more detailed stability analysis of the modified quantum walk search on hypercube with qudit walk-coin [5]. We show that in the space spanned by the walk-coin parameters there exists a relatively large high robustness area for this algorithm. We numerically check that for coin register with size up to eleven. We use deep neural network simulations to predict the algorithm's behavior for larger coin register size.

This work was supported by the Bulgarian Science Fund under contract KP-06-M48/2 /26.11.2020.

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Error correction of a logical grid state qubit by dissipative pumping

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Stabilization of encoded logical qubits using quantum error correction is key to the realization of reliable quantum computers. While qubit codes require many physical systems to be controlled, oscillator codes offer the possibility to perform error correction on a single physical entity. One powerful encoding for oscillators is the grid state or GKP encoding [1-3], which allows small displacement errors to be corrected. Here we introduce and implement a dissipative map designed for physically realistic finite GKP codes which performs quantum error correction of a logical qubit implemented in the motion of a single trapped ion. The correction cycle involves two rounds, which correct small displacements in position and momentum respectively. Each consists of first mapping the finite GKP code stabilizer information onto an internal electronic state ancilla qubit, and then applying coherent feedback and ancilla repumping. We demonstrate the extension of logical coherence using both square and hexagonal GKP codes, achieving an increase in logical lifetime of a factor of three. The simple dissipative map used for the correction can be viewed as a type of reservoir engineering, which pumps into the highly non-classical GKP qubit manifold. These techniques open new possibilities for quantum state control and sensing alongside their application to scaling quantum computing.

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How Nature covers its Bases

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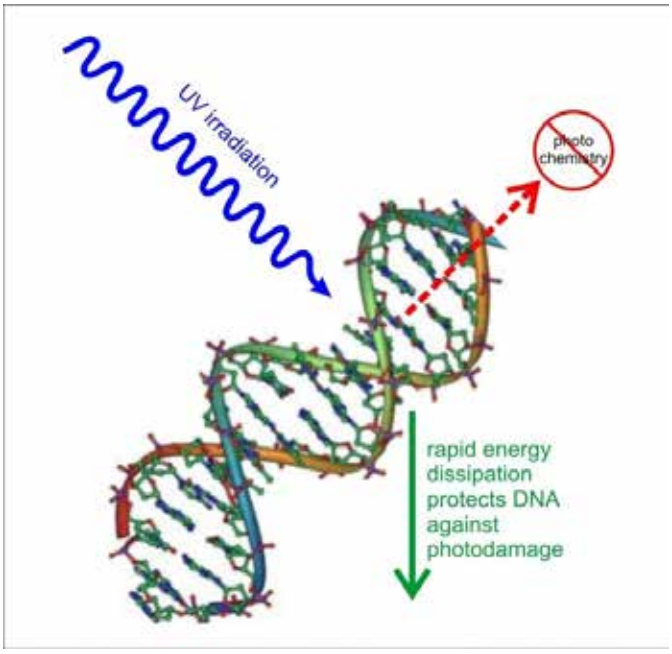
We study the interaction of molecules with light. History's great painters studied the magic of light and color by choosing pigments to tell a story in a painting. However, as skilled as they were, the Great's could not always prevent the fading of their work in time. We study why their paintings fade and suggest that art is actually imitating life.

The biochemical building blocks are also prone to degradation when exposed to light. So, we also study how one of the greatest painters of all time, nature, chose the pigments necessary in the painting of life, the bases of our DNA. Most of the heterocyclic compounds that today are involved in replication exhibit enhanced UV photochemical stability by virtue of sub-picosecond excited state life-times. The mechanism involves rapid internal conversion back to the electronic ground state through conical intersections and is exquisitely sensitive to molecular structure. This suggests the possibility of a photochemical selection of the molecular building blocks of life, as we know it, long before the advent of biological selection. It is thus conceivable that the molecular properties of nucleobases, which we study now, are relics from prebiotic chemistry that occurred 4 billion years ago: molecular fossils of prebiotic chemistry.

We explore this excited state photodynamics with REMPI, IR-UV double-resonant, and pump-probe spectroscopy in combination with ab initio modeling, in the nanosecond and picosecond time domains. We investigate isolated nucleobases, nucleobase derivatives, nucleosides, and their clusters with each other, as base pairs, and with water. From these studies an increasingly detailed picture of nucleobase excited state dynamics is now emerging



Attosecond Spectroscopy of Small Organic Molecules: XUV pump-XUV probe Scheme in Glycine

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The availability of coherent light sources with attosecond resolution (1 as=10^{-18} s) has opened the door to resolve electron dynamics in excited and ionized complex molecules. The early electron dynamics triggered in a biomolecule is at the heart of biological processes which are essential to life. Therefore, understanding the ultrafast charge dynamics that steer these processes has become a hot topic in the field of attosecond science. Attosecond time-resolve experiments allow us to retrieve images of this charge dynamics in molecules. The first experiment retrieving a sub-femtosecond ultrafast dynamics in a biomolecule was performed by using an as UV-pump/ fs IR-probe scheme in phenylananine [1]. The sub-fs charge fluctuations where associated with electronic coherences initiated by the as pump pulse. Theorical calculations to describe this experiment were initially performed considering that the nuclei of the molecule remained fixed in space [1], [2]. How long these electronic coherences can survive when nuclear motion comes into play is a question that has yet to be solved.

In the present study, we pursue to shed some light on this matter by theoretically describing the outcome of an attosecond two-color XUV-pump/XUV-probe scheme in glycine. The broadband pump pulse ionizes the molecule, creating a coherent superposition of cationic states, which evolve in time coupled to the nuclear motion until it is probed by the second XUV pulse. An explicit evaluation of the full-electron wave function in the continuum and the inclusion of non-adiabatic effects are carried out [3]. Both aspects have been addressed in this work by combining a multi-reference static-exchange method and a surface hopping approach, respectively. We have found that, in the absence of the probe pulse, ionization can lead to fragmentation of the glycine cation through the C-C or the C-N bonds. The lower electronic states of the cation are more likely to induce elongation of the C-C bond, while the higher excited states favor elongation of the C-N bond, both of which can ultimately break. Besides, we observe that by simply varying the central frequency of the pump pulse by a few eVs, one can alter the cation dynamics favouring specific fragmentation pathways. This dynamics can be probed with a second XUV pulse that further ionizes the cation. A trajectory-based analysis, employing a multireference static exchange DFT approach in combination with Surface Hopping, is employed to retrieve the dication fragmentation yields as a function of the pump-probe delay.

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S1-P34

MODELING EXCITED STATES AND RAMAN SPECTRA PROPERTIES FOR CAROTENOID WITH COMPLEXES

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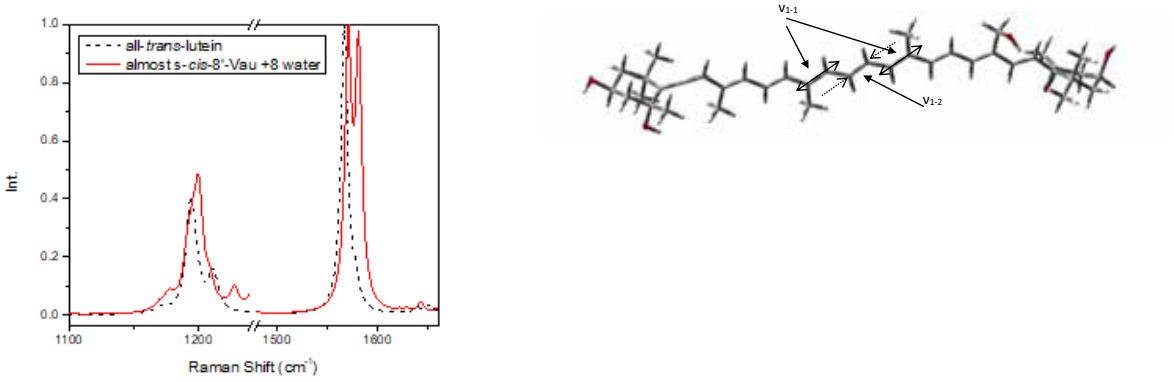
Carotenoids (Cars) have linear conjugated isoprenoid chain which affords them an intense absorption in the blue-green range. This leads that they give main contribution to colors of fruits, flowers and animals. In photosynthetic organisms, they are implicated in the harvesting of solar photons while natural carotenoids display a large structural diversity, and more than 1100 molecular species have been now identified. There are more than several photophysics models of Cars. They all are used to interpret the excited state dynamics of Cars with Chls, containing Qy and Qx states, and this shows that it is more complicated than it can be expected. Additional states for the red absorption shift is proposed to arise from an intramolecular charge transfer (ICT) character of the second excited state, generated by the electron-rich keto group also [1-3]. Large scale computations provide more detailed information which allow better understand carotenoid properties which can be expected in real life biological systems. The Car was chosen vaucheriaxanthin, fucoxanthin, lutein, beta-carotene and diadinoxanthin. All structures were optimized separately. Careful orbital analysis allowed us to label each calculated excited states. Study was done using a combination of Raman and absorption spectroscopy and density functional theory (DFT) modelling, including Car–Parrinello molecular dynamics (CPMD) simulations as it is implemented in NwChem package together with PACKMOL software.

The Cars specific bond were analyzed by suing energetic surface scan methodology by fixing all the other atoms. This methodology allows to identify additional local minima as possible conformers (Fig. 1). Using such unstable structures, they were studied by changing local environments such as with water models (Fig. 1). The stabilized new structures provide new properties in excited states or Raman activities (Fig. 1) in various Cars. In order to find stability of investigated structures the CPMD simulations are performed. Additional results with Fx suggest that due to fluctuations and interactions with the environment the new conformers can appear what can participate in explaining the SCT states in Cars.



A B

FIG. 1: Vaucheriaxanthin and lutein Raman activity model [3]:
A – spectra; B – vibration data

Acknowledgements

M.M. and L.D. acknowledges the support by Research Council of Lithuania (grant no. S-MIP-20-47). Computations were performed on resources at the supercomputer "VU HPC" Saulėtekis of Vilnius University in Faculty of Physics.

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Coaxial ion source: characterization of field ionization under gas flow

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An ion source with a coaxial structure [1] comprises an ultrafine tungsten tip introduced into a stainless steel capillary that joins a "high pressure" chamber (up to 1000mbar) and a very low pressure chamber (<10^{-4}mbar). After characterizing behavior of molecular flows obtained in this structure [2], we estimated that ion source had an apparent source-size <2nm [3] and that under all flow conditions. Today, we are interested in the emitted intensity for all flow conditions and for different gases: argon, hydrogen, helium, xenon,... Because of residual water the tip is transformed, tungsten is corroded under the electric field. Traces of water are measured by mass spectrometry and confirm these results. The intensity emitted as a function of the voltage depends strongly on the tip shape. The monitoring of the characteristics I(V) as a function of the size of the tip will be presented. This approach allows a better understanding of the mechanisms involved to model the supply function in this system.

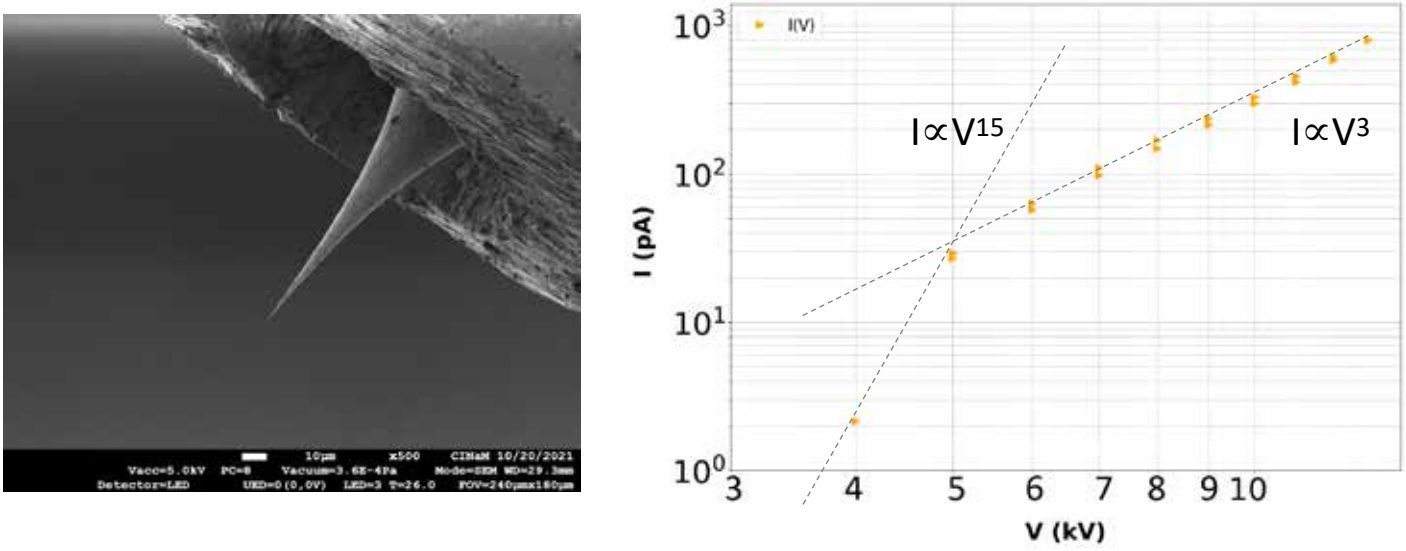

FIG. 1: Left: Coaxial ion source observed under scanning electron microscope. Right: Ionization intensity versus voltage characteristic obtained for P=10^{-5}mbar in the low pressure chamber.

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Quantum Simulation of the Central Spin Model with a Rydberg Atom and Polar Molecules in Optical Tweezers

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Central spin models, where a single spinful particle interacts with a spin environment, find wide application in quantum information technology and can be used to describe e.g. the decoherence of a qubit over time. We propose a method of realizing an ultracold quantum simulator for the central spin model. The proposed system consists of a single Rydberg atom ("central spin") and surrounding diatomic molecules ("environment spins"), coupled to each other via dipole-dipole interactions. By mapping internal particle states to spin states, spin-exchanging interactions can be simulated. We demonstrate that this setup allows realizing a range of central spin models of high scientific interest. More precise control over the model can be exerted by directly manipulating the placement of environment spins. As an example, we consider a ring-shaped arrangement of environment spins, and show how the time evolution of the central spin is affected by the tilt angle of the ring.

Exploiting quantum interference to increase efficiency and power of solar cells

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Quantum interference is a quantum process whose effects range from changing optical properties of media, like absorption and transparency, to enhancing energy transport in light-harvesting complexes or information transfer in quantum networks. This process can arise through the application of coherent fields or, more surprisingly, even through incoherent processes like spontaneous emission [**1**].

Solar cells could see improvements in their performances exploiting quantum interference between internal states. Using a V-type three-level system to model a photocell, Svidzinsky *et al.* demonstrate theoretically in [**2**] that the cell, if excited by natural incoherent light, *i.e.* sunlight, can experience quantum interference involving the transitions from a common ground state to the excited states. The phenomenon leads to a mitigation of radiative recombination and thus to a significant increase in photocurrent and electric power that can be extracted from the cell.

Starting from this model, we propose an experiment realizing a V-type three-level system in the hyperfine structure of Rb atoms. Similar to [**3**], the aim of our proposal is the observation of quantum beats in the spontaneous emission spectrum from hot Rb atoms, driven by an incoherent field, that proves the presence of quantum interference. This is expected to provide us new insight about quantum coherence terms originated by non-coherent excitation, like solar radiation, that could be exploited in the future for novel high-efficiency solar cells.

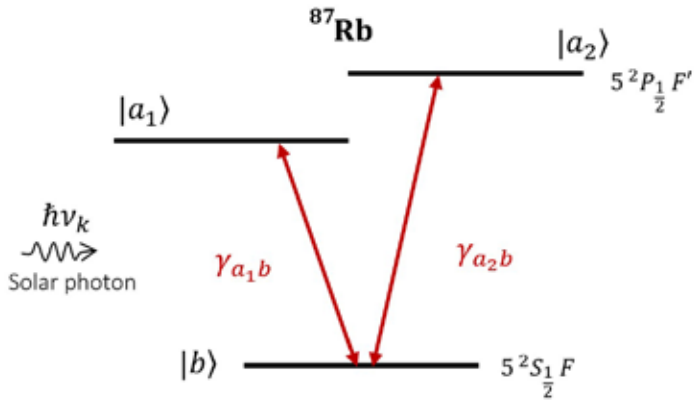

FIG. 1: V-type three level system in the ^{87}Rb D_1 transition hyperfine structure. The incoming photon of mode ν_k, close to the transition frequencies, promotes the electron in one of the two excited states. Rates γ_{a_1b}, γ_{a_2b} are the spontaneous emission rates.

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Probing Dynamics in PMMA via Transient Absorption Spectroscopy

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Transient Absorption Spectroscopy (TAS) [1] is a well-established technique that has been extensively applied to investigate the dynamics associated with photophysical and photochemical reactions in various compounds in liquid phase (e.g. photosynthetic systems [2] and organometallics [3]). In this work, we present TAS preliminary spectroscopic measurements in Polymethylmethacrylate (PMMA) dissolved in Dichloromethane (DCM).
A thorough understanding of the dynamics in PMMA is important due to its key role as a resist material in the field of Extreme-UV Lithography (EUVL) [4,5], a field with significant socio-economic impact. Figure 1 shows a kinetic trace at a wavelength of 772 nm following excitation with a 400 nm pump wavelength. A decay with a lifetime of 56 ps was extracted by means a global analysis performed using the Glotaran software. Further experiments and analysis are ongoing.

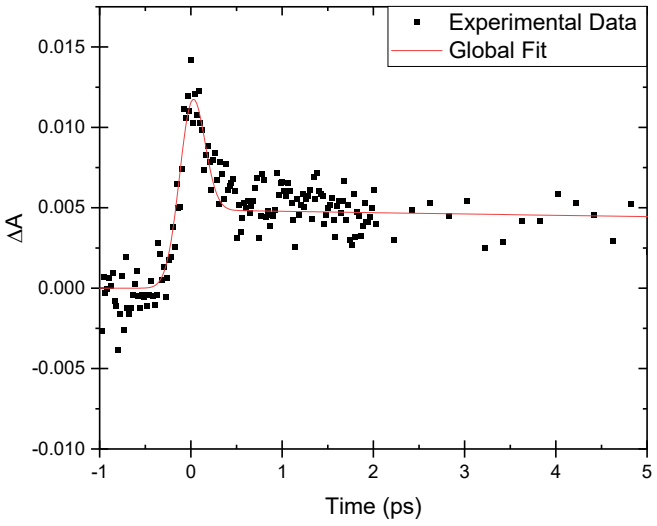

FIG. 1: Time trace at 772 nm, fitted with a 56 ps decay.

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Spin squeezing in the two-component Bose-Hubbard model with long-range interactions

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We study a generation of spin-squeezing with ultra-cold atoms in two internal states loaded in an one-dimensional optical lattice with unit filling. We describe the system by the two-component Bose-Hubbard model taking into account short and long range interactions. The atoms are initially in the spin coherent state in the superfluid phase delocalized over the entire lattice. In the absence of long-range interactions, the quantum dynamics of the system is well captured by the one-axis twisting model. In general case, the zero-momentum part of the system Hamiltonian leads to the anisotropic two-axis counter twisting model. We study the scaling of the best squeezing and the best squeezing time with the number of atoms from the resulting model and show that Heisenberg-limited squeezing is possible in a wide range of anisotropy.

Momentum-map analysis of strong-field double ionization in three-electron atom

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We study double ionization of a three-active-electron atom model with partially antisymmetric spin structure (two spins up, one spin down) using the recently developed numerical code that allows one to simulate multiple ionization in momentum space without loss of high energy electrons [1]. We have found that the correlation of the famous V-structure in two-electron momentum map [2] and direct ionization channel is evident by simultaneous inspection of momentum distributions and ionization yield values for different channels, without employing any classical analogies at all. Besides, we investigate the dependence between two-electron momentum maps symmetry and intensities of different double ionization channels; such a dependence can serve as a valuable source of ionization dynamics information. Understanding main properties of two-electron momentum distribution opens a path to creating a composite model for double ionization of three-electron atom that combines a number of technically two-electron models.

The simulations were performed with use of the facilities of PL-Grid Infrastructure. This work was realized under National Science Centre (Poland) project Symfonia No. 270 2016/20/W/ST4/00314.

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S1-P42

Vibrational high resolution spectroscopy of biomolecules in a cryogenic 16-pole wire ion trap

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Spectroscopy plays an increasingly important role in the study of structural details of complex biological systems and the investigation of UV photodamage of e.g. the monomers of the genetic material. In combination with electrospray ionization, ion trap spectroscopy has been successfully used to investigate electronic and vibrational transitions in biological molecules, to understand geometrical structures or the decay channels of electronic excitation. [1,2]

In this contribution a recently developed linear cryogenic 16-pole wire ion trap for ion spectroscopy at temperatures below 4K will be presented. The trap offers a large field-free region in the radial direction, reducing radio-frequency heating and also a large optical access perpendicular to the ion beam direction. Effective trapping potential of the wire-based radio frequency trap will be shown and compared to conventional multipole ion trap designs. [3]

The low temperatures of the wire trap enabled binding of up to four helium atoms on protonated glycine ions. From temperature-dependent ion intensities an activation energy for collision-induced dissociation is derived and will be presented. With a pulsed infrared laser the OH stretching vibration by vibrational predissociation spectroscopy of trapped $GlyH^+(He)_n$ (n = 1 to 3) has been studied, where only small shifts of the center frequency have been observed. The width of the absorption peak, was fitted with a simulated rotational contour yielding a rotational temperature of about 6K. [4] Finally, preliminary results of UV photodissociation studies of $[dAMP\text{-}H]^-$, a monomer of the DNA, will be presented.

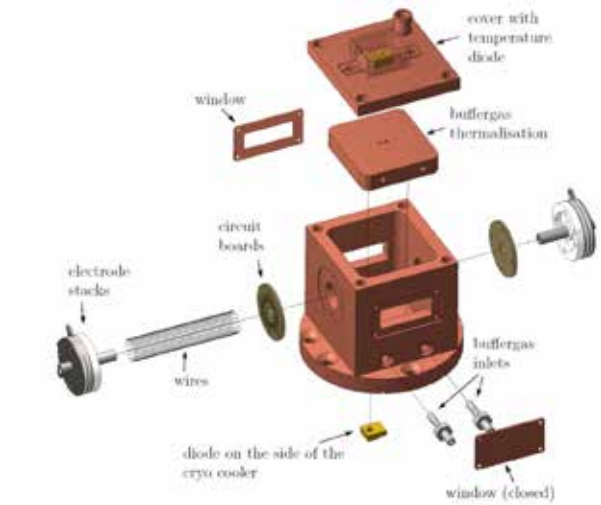

FIG. 1: Schematic of the cryogenic 16-pole wire ion trap.

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Studies of the First Excited $^1\Pi$ State in Cs-containing Alcali Diatomics

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The Cs-containing polar alcali diatomic molecules NaCs, RbCs, and KCs possessing sufficiently large values of permanent electric dipole moments are attractive objects of research for producing in ultracold conditions. In this connection there is a growing interest in detailed high-accuracy experiment-based information on the excited electronic states converging to the first excited atomic asymptote states, which are the $A^1\Sigma^+$, $b^3\Pi$, $c^3\Sigma^+$ and $B^1\Pi$. The main current strategy is to involve the states in a deperturbative analysis of the strongly mixed (mutually perturbed) $b^3\Pi$, $c^3\Sigma^+$ and $B^1\Pi$ states referred to as a '*B-b-c* complex'. In this contribution we present an overview of experimental data on the $B^1\Pi$ state of NaCs [1], RbCs [1, 2], and KCs [3, 4] obtained from *B-X* fluorescence spectra dispersed by Fourier-Transform spectrometer with a typical spectral resolution 0.03 cm^{-1}. It should be noted that the more abundant systematic $B^1\Pi$ state of NaCs data have been obtained in [5] by two-colour polarisation labelling spectroscopy. In all cases the $B^1\Pi$ state appears to be heavily perturbed even for rather low *v'* values of vibrational quantum numbers. Because of lack of information about the perturbing states, in particular on the $c^3\Sigma^+$ state, it was only possible to select the less perturbed term values to be involved in a single-state spline-pointwise potential construction. Presently with appearance of detailed spectroscopic information on the $c^3\Sigma^+$ state [6, 7] the numerous amount of data on perturbed levels becomes important and will necessarily be involved in depertubative treatment. Additional experimental data on the Lambda – doubling constant and the *J*-dependence of the rotational constant are analysed.

The work was supported by the Latvian Council of Science, project No. lzp-2018/1-0020: "Determination of structural and dynamic properties of alkali diatomic molecules for quantum technology applications".

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Laser Photodetachment Studies in a Storage Ring and Application to Mass Spectrometry

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Negative ions play an important role in high sensitive mass spectrometry. Notably accelerator mass spectrometry (AMS) depends strongly on negative ions due to its use as a selective filter. Laser photodetachment of negative ions can be used as an additional element selective filter to suppress atomic or molecular isobars. To this end, photons interact with the negative ions and remove the extra electron if the photon energy exceeds the electron affinity (EA) of the negative ion. As the EA solely depends on the electron configuration this process is element selective.

For most atomic negative ions the EA is well known. However, in the case of molecular negative ions this is not the case. Especially for AMS relevant molecules the lack of spectroscopic information of molecular negative ions is evident. One reason for this are the internal degrees of freedom of molecules. In that case more effort has to be taken in gathering the required spectroscopic information. One possibility is the use of low–energy storage rings, where the internal degrees of molecules can be cooled during storage. Recently, the electrostatic storage ring FLSR [1] was equipped with a negative ion source. Photons from a high–repetitive tuneable Ti:sapphire laser are directed to one of the interaction point of the storage ring, which was equipped with optical grade vacuum windows. The neutralised particles are further downstream detected with a position–sensitive silicon strip detector. By varying the laser wavelength the detachment threshold of the negative ion and therefore the EA can be studied. First tests have been performed with stored oxygen anions and show promising results. Further tests with molecular hydroxide anions will be performed. In a later stage of the project, a sputter ion source will be used to produce the molecules relevant for mass spectrometry.

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High-Resolution Dielectronic Recombination Spectroscopy with Slow Cooled Pb^{78+} Ions in the CRYRING@ESR Storage Ring

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Dielectronic Recombination (DR) spectroscopy is a widely used and very successful technique to study the properties of highly charged ions [**1**–**3**]. Its high precision and versatility make it an important spectroscopic tool in the physiscs program of the SPARC collaboration, e.g. outlined in the CRYRING@ESR Physics Book [**4**]. The range of accessible topics encompasses the measurement of input data for plasma modelling and astrophysics, the investigation of nuclear properties, as well as tests of QED in strong fields and lifetime studies.

The heavy-ion storage ring CRYRING@ESR of the international FAIR facility in Darmstadt is a very attractive machine for performing DR spectroscopy because of its electron cooler that is equipped with an ultra-cold electron beam promising highest experimental resolving power and because of the extreme versatility of the storage ring ESR as its injector. Here, we report on results from the first DR experiment with highly charged ions at this new facility.

The measured DR spectra of Pb^{78+} in the collision energy range of 0–40 eV cover the $2s2p\ (^3P_1)\ 19\ell$ and $2s2p\ (^3P_1)\ 20\ell$ resonances resulting from electron capture of the Be-like core: $2s^2\ ^1S_0 \rightarrow 2s2p\ ^3P_1$. While the analysis of data is still ongoing, the preliminary results show good agreement of relative peak positions and peak strengths with theoretical calculations using the methodology described in Ref. [**5**].

Furthermore, the comparison between experiment and theory shows that the experimental resolving power is according to the expectations. For kinematic reasons the resolving power of electron-ion merged-beams experiments is highest at the lowest electron-ion collision energies. We will exploit this in future high-resolution studies with few-electron heavy ions which exhibit DR resonances at energies below 1 eV as, e.g., Xe^{50+} [**6**].

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Topological Aspects of Quantum Light-Induced Conical Intersections

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Abstract Conical intersections (CIs) are degeneracies between multidimensional potential energy surfaces of molecular systems. It is well known that their presence in a molecular system has noticeable nonadiabatic topological implications. Such a consequence is the appearance of the topological or geometric phase. CIs can also be created by classical laser light or by quantum light in an optical cavity (light-induced conical intersections, LICI). We discuss LICIs : a) between electronic polaritonic surfaces [1] as well as b) between vibrational polaritons [2]. It is demonstrated that in both cases the topological properties of the studied molecules show clear fingerprints of the nonadiabatic couplings between the electronic, vibrational/rotational and photonic modes of the systems.

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Compact 3-D Caesium Vapour Magnetometer

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We present a compact magnetometer that measures the magnetic field along 3 axes using two beams from the same laser. We follow the approach proposed by LeGal *et al.* [1] using a pump beam to create atomic alignment that interacts with the magnetic field in two directions and is measured by a polarization-modulated probe beam but apply it to Caesium vapour and add a radio-frequency (RF) double resonance measurement to determine the third component of the magnetic field. The principle of alignment magnetometry is illustrated schematically in Fig. 1. The linearly polarized pump beam with polarization vector $\vec{E_p}$ creates alignment of atomic angular momentum $\vec{d}$ along the z-axis. The x-component of magnetic field will cause Larmor rotation of the aligned angular momentum $\vec{d}$ in the zy-plane [Fig. 1(a)]. Similarly, the y-component of the magnetic field causes rotation in the xz-plane [Fig. 1(b)]. The linearly polarized probe beam is modulated by an electro-optic modulator (EOM) so that its electric field vector lies in the yz-plane for measurements of $\vec{B_x}$ or the xz-plane for measurements of $\vec{B_y}$. The Larmor rotation will alter the relative alignment of the atomic angular momentum $\vec{d}$ with the probe beam polarization ($\vec{E_x}$ or $\vec{E_y}$), which leads to the dispersion signals shown schematically next to the geometry. The RF coils are added with their axis along the z-direction to measure the z-component of the magnetic field. The approach is simple to implement because the angle between pump and probe need not be large and so they can use the same optical windows.

In addition, we are rewriting the computer code used to model these interactions using the QuantumOptics.jl framework of the Julia language [2]. This code will be easier to maintain and share compared to the current version, written in C/C++. Julia is almost as fast as C/C++, and allows for easy parallelization, reducing computation times from days to hours or even less, depending on the number of cores available.

We will present the progress made on our experimental measurements and theoretical modelling.

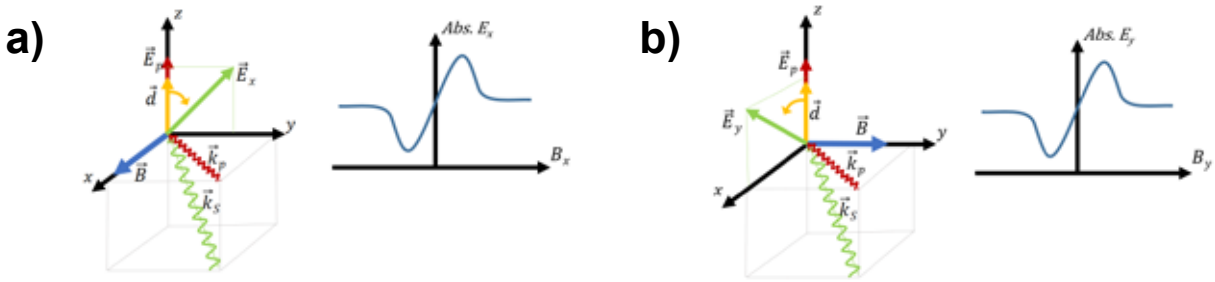

FIG. 1: Geometry and signal for alignment magnetometry for (a) $\vec{B_x}$ and (b) $\vec{B_y}$.

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Continuous measurement of a quantum system

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We introduce a model of repeated position and momentum measurement of a single quantum particle. The particle is considered an open system in an environment of detectors, described by a Lindblad equation. Using the Monte Carlo wavefunction method allows us to predict single trajectories. In the poster I present the emergence of different types of such trajectories: classical and Zeno-like dynamics.

Intracavity Rydberg superatom for optical quantum engineering

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We present several key steps towards quantum engineering of light on a new experimental platform capable of creating strong interactions between optical photons [1]. This platform is based on a small (5 µm rms) and cold (2 µK) rubidium ensemble with a strong collective coupling to a single-ended medium-finesse running-wave resonator. A bright control laser couples the excited atomic 5P state to a long-lived Rydberg state, creating an Electromagnetically Induced Transparency (EIT) effect and mapping intracavity photons to Rydberg polaritons. The van-der-Waals interactions between the latter lead to strong optical nonlinearities such that the propagation of photons through the cavity becomes very dependent on the Rydberg population. We experimentally verified that in our system these interactions are strong enough for the presence of one Rydberg atom to block the excitation of others. This leads to a strong antibunching between photons transmitted through the cavity when the system is driven on resonance. Off-resonant driving can reverse this effect and lead to photon bunching.

In this strong blockade regime, the atomic ensemble behaves as a single Rydberg superatom strongly coupled to the cavity. We can coherently drive two-photon Rabi oscillations between its ground state $|G\rangle$ and its collective singly-excited Rydberg state $|R\rangle$, and observe a collective enhancement of its frequency confirming the effect of the Rydberg blockade. The state-dependent transmission of the cavity allows us to detect the state of the superatom in a single shot with a 95% efficiency. The switching contrast between the two transmission levels is ~ 20, significantly higher than for free-space Rydberg ensembles.

Finally, we show that by carefully tuning and optimizing our experimental parameters we reached a regime where rotating the state of the superatom from $|G\rangle$ to $|R\rangle$ changes the optical impedance of the cavity from strongly over- to strongly under-coupled, thus inducing a π phase shift on the light reflected off of it (see Fig. 1). This conditional phase shift allows us to detect the state of the superatom with a 90%efficiency via a homodyne measurement. Together with the coherent control and the single-shot state detection, it is a key ingredient for the implementation of an efficient controlled-phase gate or for the deterministic generation of optical "Schrödinger's cat" states without the need for a low-volume high-finesse cavity.

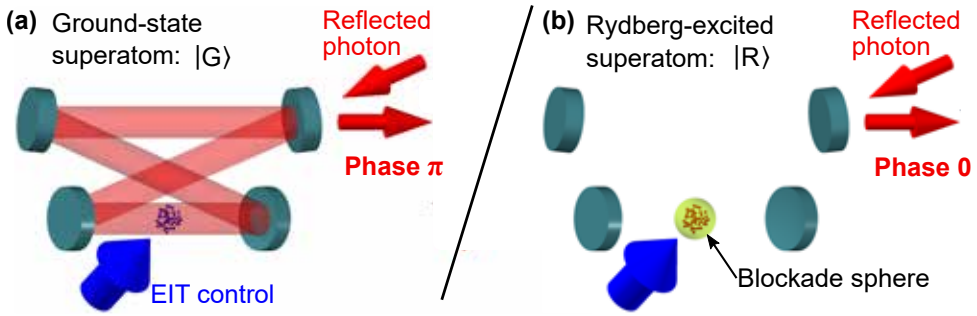

Figure 1: Superatom state-dependent optical π phase shift. (a) When the superatom is its ground state $|G\rangle$ (all atoms in their ground state), the Rydberg Electromagnetically Induced Transparency (EIT) enables a resonant dark polariton mode. A reflected photon enters the cavity and comes out with a π phase. (b) With a single Rydberg collective excitation present in the atomic cloud (state $|R\rangle$), the strong interactions between Rydberg atoms blockade the EIT and the corresponding resonant mode. A photon is then directly reflected with a zero phase.

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Measuring the Casimir-Polder Rydberg-surface interaction by vapour cell spectroscopy

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The modification of quantum fluctuations by a surface of finite reflectivity shifts the energy levels of atoms (Casimir-Polder effect). At nanometric distances away from a surface (near field), the Casimir-Polder shift is given by $-C_3/z^3$ (where C_3 is the van der Waals coefficient and z is the atom-surface distance) corresponding to the interaction of the fluctuating atomic dipole with its surface-induced image. Rydberg-surface interactions are of fundamental interest because the atomic size, scaling as n^{*2} (where n^* is the principle quantum number corrected by the quantum defect), is no longer negligible compared to the atom-surface separation. In this case, the interaction of the fluctuating atomic quadrupole (higher-order terms) with its own image needs also to be taken into account. The distance dependence of quadrupole interactions is predicted to be z^5 [1] but has not been experimentally investigated yet.

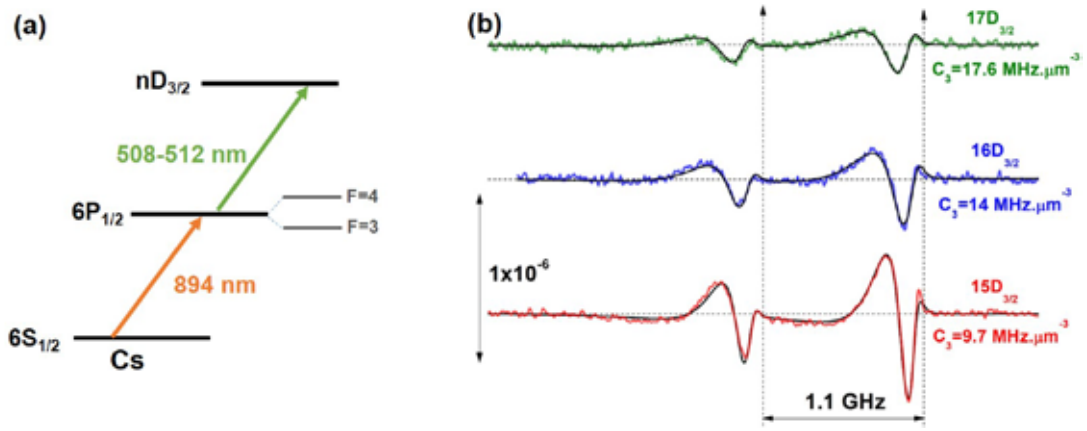

Figure 1: (a) Relevant cesium energy levels. (b) Normalised selective reflection spectra (black lines) for the $6P_{1/2} \rightarrow nD_{3/2}$ transitions (where n=15,16,17) at 25mTorr pressure. Theoretical fits are represented with coloured lines. The two peaks correspond to the $6P_{1/2}$ hyperfine manifold separated by 1.1 GHz [2]

We use selective reflection spectroscopy that probes atoms at nanometric distances away from a vapor cell window and allows us to measure the Casimir-Polder interaction between Cs($nD_{3/2}$) (where n=15-18) atoms and a sapphire surface. Our set-up is similar to the one reported in [2]. Cesium atoms are excited to the first cesium resonance ($6P_{1/2}$) and subsequently selective reflection is performed on the $6P_{1/2} \rightarrow nD_{3/2}$ transition (see Fig.1a). We interpret our experimental spectra using a theoretical model that neglects the effects of atomic motion (justified when the Casimir-Polder shift is much larger than the Doppler shift). The experimentally extracted values of the C_3 coefficients scale with the principle quantum number as n^{*4} (as expected) but remain slightly larger then elementary theoretical predictions.

We are currently improving our theoretical models to extract more precise measurements of the C_3 coefficient. We are also conducting experiments on a thin cell [3], which allows us to control atom-surface distances and test the limits of the dipole approximation. We thank the ANR (ANR-20-CE92-0006-0.1) for financial support.

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Rovibrational dynamics of a diatomic molecule in an optical centrifuge

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We present a theoretical study of the rotational and vibrational dynamics of a diatomic molecule in the electric field produced by an optical centrifuge. The time-dependent Schrödinger equation is solved by including a time profile of the optical centrifuge similar to the experimental laser pulse used by the experimental group of V. Milner [**1**]. Taking as prototype Rb_2 molecule, we investigate the field-dressed dynamics of rovibrational states within the electronic state $a^3\Sigma$ considering peak intensities of the order of 10^{11} W/cm^2.

After the laser pulse, a significant population from the initial wave packet is transferred to other vibrational bands, which indicates that the rigid rotor approximation is no longer valid for this laser field regime. Moreover, in some cases, there is a large fraction of population going into the continuum, which might be greater than 30%, indicating the dissociation of the molecule. By decreasing the laser intensity, transitions to other vibrational states as well as to the continuum are reduced. We find a rather small population transferred ($\lesssim 0.02\%$) to the continuum with $I_0 \lesssim 1\cdot 10^9$ W/cm^2, $\beta = 0.3$ fs^{-2} and the initial states $\nu_0 = 30$, $J = 0$ and $\nu_0 = 35$, $J = 0$.

These results are compared with those obtained from a laser pulse having the same turning-on and turning-off profiles, but constant intensity between them. For this pulse, a similar set of vibrational bands, but with a different weight, are populated. However, the population transferred into continuum is even larger for the same peak intensity. This can be explained in terms of the energy absorbed by the molecule, which is larger than with the centrifuge pulse.

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Universality in three-body collisions of ultracold hybrid ion-atom systems

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We introduce the concept of universality: a tool for efficient description of the scattering properties of ultracold three-body systems. We discuss the motivations behind implementing universal potential models in order to calculate the recombination losses in ion-atom samples. We will proceed to showing how we can model an exemplary three-particle collision in a system interacting via the sum of two-body potentials. The poster presentation includes a reference to recent theoretical results in hybrid systems of Barium [1] and Ytterbium [2] ions immersed in Lithium gas – where recently Feshbach resonances between a single ion and ultracold atoms were observed. I shall show the limits of the universal approach in ion-atom systems: mainly the difficulties in proper description of weakly bound states as well as the differences in treating the atom-atom and atom-ion channels of scattering.

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Single-Atom Heat Engine as a Sensitive Thermal Probe

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We propose utilizing the single-atom heat engine [1] as a sensitive probe for thermal baths. This engine runs in an open Otto cycle, allowing for the accumulation of oscillation in a flywheel. The sensitivity of this scheme is estimated, using analytical and numerical modeling, to be able to detect temperature differences as small as 2 μK. This method can be employed without requiring a quantum state initialization with a wide range of base temperatures. A further enhancement of the sensitivity can be realized by employing quantum resources, such as squeezing of the motion of the ion [2]. Furthermore, we report on the recent experimental advances in our setup.

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N Impenetrable Particles Bouncing on a Mirror: Discrete Time Crystals

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Spontaneous time-translation symmetry breaking had not attracted much attention until Wilczek [1] introduced the concept of time crystals. Despite this particular realization being prohibited by the ,,no-go" theorem [2], the idea inspired a new version of time crystals, i.e. the discrete time crystals (DTCs) [3]. In general, a DTC is a periodically driven quantum many-body system that spontaneously breaks the discrete time-translational symmetry of the Hamiltonian due to particle interactions and starts evolving with a period s-times longer than the period of the external driving.

In our previous works, we developed a theoretical basis for the realization of DTCs in the ultra-cold atom platform, i.e. a Bose-Einstein condensate (BEC) of weakly interacting bosonic atoms bouncing resonantly on a periodically driven atom mirror in a 1D space [3–5]. In our present work we take that idea further, and consider a collection of BECs.

Here we shall present the first stage of our analysis. It constitutes a classical basis for quantum research of novel time crystal and condensed matter phenomena in the time domain. We consider the dynamics of N impenetrable particles (hard balls) of equal masses stacked above each other in a 1D space. The particles bounce on an oscillating mirror in the presence of gravitational field. We identify the manifolds the particles move on and derive the effective secular Hamiltonian for the resonant motion of the particles. The effective Hamiltonian can be interpreted as describing a fictitious particle in an N-dimensional effective potential (N-dimensional particle) [6].

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Polyatomic ultralong range Rydberg molecules

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In cold and ultracold mixtures of atoms and molecules, Rydberg interactions with surrounding atoms or molecules may, under certain conditions, lead to the formation of special long-range Rydberg molecules [**1**, **2**, **3**]. These exotic molecules provide an excellent toolkit for manipulation and control of interatomic and atom-molecule interactions, with applications in ultracold chemistry, quantum information processing and many-body quantum physics.

In this poster, we discuss ultralong-range polyatomic Rydberg molecules formed when a heteronuclear diatomic molecule is bound to a Rydberg atom [**3**, **4**]. The binding mechanism appears due to anisotropic scattering of the Rydberg electron from the permanent electric dipole moment of the polar molecule. We propose an experimentally realizable scheme to produce these triatomic ultralong-range Rydberg molecules in ultracold KRb traps, which might use the excitation of potassium or rubidium [**5**]. By exploiting the Rydberg electron-molecule anisotropic dipole interaction, we induce a near resonant coupling of the non-zero quantum defect Rydberg levels with the KRb molecule in an excited rotational level. This coupling enhances the binding of the triatomic ultralong-range Rydberg molecule and produces favorable Franck-Condon factors.

Another type of ultralong-range Rydberg molecule is formed in collisions between polar molecules in cold and ultracold settings [**6**]. The interaction of Λ-doublet nitric oxide (NO) with long-lived Rydberg NO molecules forms ultralong-range Rydberg bimolecules with GHz energies and kilo-Debye permanent electric dipole moments. The description includes both the anisotropic charge-molecular dipole interaction and the electron-NO scattering. The rotational constant for the Rydberg bimolecules is in the MHz range, allowing for microwave spectroscopy of rotational transitions in Rydberg bimolecules. The Rydberg molecules described here hold promise for studies of a special class of long-range bimolecular interactions.

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A comb-calibrated deep-ultraviolet laser spectrometer for temperature metrology

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Doppler Broadening Thermometry (DBT) is one of the primary methods of gas thermometry considered for the practical realization of the new kelvin [1, 2]. In its best implementation, performed in a gas of acetylene, the thermodynamic temperature was determined with a global relative uncertainty of about 20 ppm [3]. Here, we report on the status of a new DBT experiment that can further reduce this uncertainty, based upon the precise observation of the shape of the intercombination transition ($6s^2$ $^1S_0 \rightarrow$ 6s6p $^3P_1$ at 253.7 nm) of mercury vapors, by using a comb-calibrated laser spectrometer.

Deep-UV coherent radiation is produced through a double-stage second-harmonic generation (SHG) process, starting from the output radiation of an external-cavity diode laser at 1014.9 nm [4]. After a single passage through a periodically-poled lithium niobate crystal, the near-infrared radiation is converted into green light at 507.4 nm and used for injection locking of a high-power diode laser. Then, a second SHG process generates the 253.7 nm radiation through a BBO crystal placed inside a resonant cavity, employing the common bow-tie design. The realized source shows over 16 GHz mode-hop-free tunable range. Laser-gas interaction takes place inside an isothermal cell, showing a relative temperature stability of 0.2 ppm, filled with mercury vapors [5]. The near-infrared laser is directly referenced to an optical frequency comb synthesizer (OFCS), adopting a new scheme in which the comb spectrum at 2 μm is frequency-doubled through a single pass in a MgO:PPLN crystal.

FIG. 1 shows an example spectrum of the intercombination transition recorded at 253.7 nm. Accurate frequency scans around the Hg line are obtained by continuously tuning the OFCS repetition rate, while the near-infrared laser is locked to the nearest tooth of the frequency-doubled part of the comb.

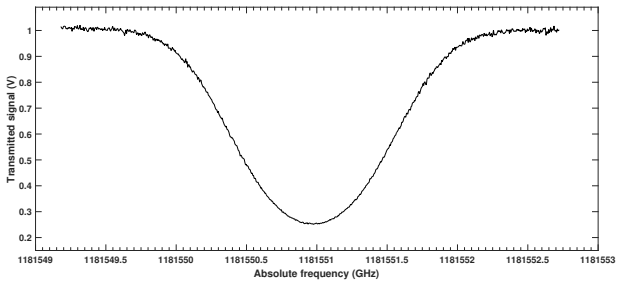

FIG. 1: ^{200}Hg absorption signal in coincidence with the intercombination transition at 273.16 K.

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Broadband Conical Third Harmonic Generation Induced by Femtosecond Filamentation in Fused Silica

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The propagation of intense femtosecond laser pulses in transparent dielectric media induces long filaments and leads to the spectacular supercontinuum (SC) generation often having ultrabroadband, several-octave-spanning spectrum [1]. Third harmonic (TH) generation is also a frequently observed nonlinear optical effect, which is produced during filamentation of infrared (IR) laser pulses with and without the onset of SC generation [2,3]. TH was reported under various experimental settings in semiconductors [4], liquids [5] and solid-state [1] dielectric media. However, TH generation is a relatively weak third-order nonlinear process due to large phase mismatch and therefore TH signal often overlaid by much more intense SC emission [1]. It was demonstrated that TH generation during IR femtosecond laser pulse filamentation in air results in both on-axis and off-axis (conical) TH components [6]. More recently, conical TH emission in various crystals and glasses produced by high repetition rate filamentation of femtosecond laser pulses was reported and it was unveiled that conical TH generation occurs as a noncollinear phase-matched four-wave mixing process [7].

In this Contribution we demonstrate that filamentation of femtosecond laser pulses leads to the generation of broadband conical TH emission during SC generation. These findings are supported by the measurements of frequency-angle spectra of filament generated in fused silica for input wavelength of 2 μm (Fig. 1(a)), which show SC spectrum with its distinct off-axis blue-peak and at larger angles conical TH emission, which covers a broad spectral range from 380 to 780 nm at different TH cone angles. The experiments were performed using wavelength tunable 160 fs pulses from an optical parametric amplifier, pumped by an amplified Yb:KGW laser at 10 kHz repetition rate. We also investigated the behavior of conical TH generation at various input beam wavelengths in the 1-3 μm range (Fig. 1(b)-(d)) and measured TH cone angles. Our experimental results are in a good qualitative agreement with the proposed model for conical TH generation, see the red curve in Fig. 1(a).

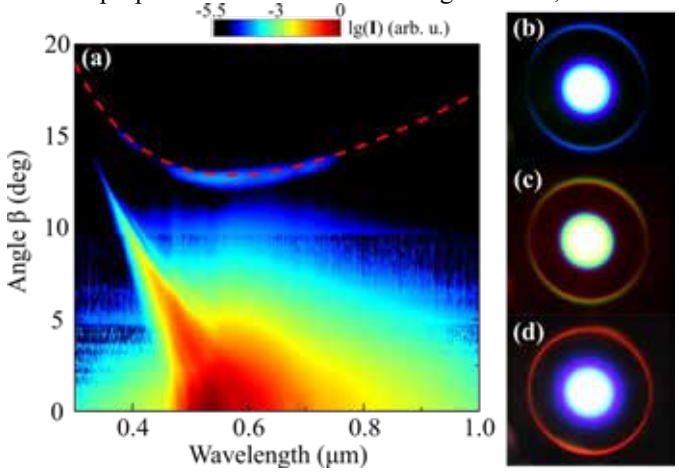

Fig. 1. (a) Experimental angularly resolved spectrum in fused silica at 2 μm. Red line indicates calculated phase-matching curve for conical TH generation. Screenshots of SC and TH emissions for input beam wavelengths of (b) 1400 nm, (c) 1700 nm and (d) 1900 nm.

We believe that our study provides a deeper understanding about the nature of conical TH generation during femtosecond filamentation and supercontinuum generation in bulk solid-state materials.

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Spin-dependent sub-wavelength optical lattices

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Traditionally, optical lattices are created by interfering two or more light beams, so that atoms are trapped at minima or maxima of the emerging interference pattern depending on the sign of the atomic polarizability [1]. Optical lattices are highly tunable and play an essential role in manipulation of ultracold atoms [2–3]. Yet the characteristic distances over which standard optical lattice potentials can change are limited by diffraction and thus cannot be smaller than half of the optical wavelength.

On the other hand, the diffraction limit does not necessarily apply to optical lattices relying on coherent coupling between atomic internal states [4–7]. It was demonstrated theoretically [4,5] and experimentally [6] that a periodic array of sub-wavelength barriers can be formed for atoms populating a long lived dark state of the Λ-type atom-light coupling scheme. The Λ scheme has a single dark state, so no spin (or quasi-spin) degree of freedom is involved for atomic motion in the dark state manifold.

In this work we demonstrate that the tripod atom light coupling scheme shown in Fig. 1 can be used to create a lattice with spin-dependent sub-wavelength barriers [8,9]. The tripod scheme is then characterized by two dark states playing the role of quasi-spin states, forming an effective brick-wall type semisynthetic lattice that can be manipulated with the relative phase of the coupling fields. Introducing a spinor degree of freedom provides new possibilities for controlling the spectral and kinetic properties of atoms in the lattice, as well as spin ordering and symmetry breaking. The tripod lattice can be realized using current experimental techniques.

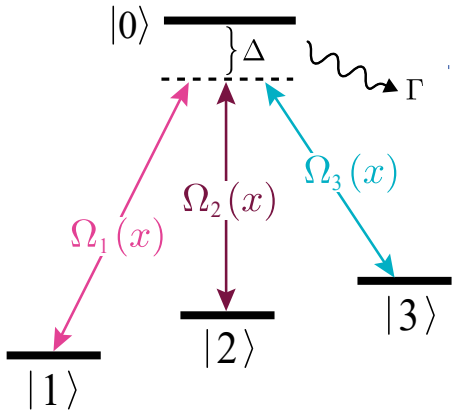

FIG. 1: The Tripod atom-light coupling scheme. Three metastable atomic ground states are coupled to an excited state via spatially-dependent Rabi frequencies $\Omega_{1,2,3}(x)$. The laser fields are detuned by Δ, and the excited state is described by a spontaneous decay rate Γ.

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Merged-beams experiments on molecular ion-neutral reactions for astrochemistry

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Gas-phase formation of complex molecular ions in the interstellar medium proceeds dominantly through barrierless ion-neutral reactions at typical temperatures of $10 - 100$ K. Our merged-beams apparatus operated at Columbia University in the City of New York enables us to measure energy-dependent absolute cross sections of molecular formation processes for reactions of singly-charged molecules with neutral atoms and derive temperature-dependent thermal rate coefficients for individual product channels. Focusing on key reactions implemented in astrochemical models as well as on systems of fundamental interest, we have recently studied the reactions

(1) $D + H_3^+ \rightarrow H_2D^+ + H$ [1],

(2) $D + H_2D^+ \rightarrow D_2H^+ + H$ and $D + D_2H^+ \rightarrow D_3^+ + H$ [2],

(3) $C + H_2^+ \rightarrow CH^+ + H$ and $C + D_2^+ \rightarrow CD^+ + D$ [3],

(4) $O + H_3^+ \rightarrow OH^+ + H_2$ and $O + H_3^+ \rightarrow H_2O^+ + H$ [4].

Our study of reactions (1) and (2) was initially motivated by questions of H_3^+ deuteration pathways in star-forming regions, but has meanwhile turned out to be a key reaction to test ab-initio quantum-mechanical calculations of molecular reaction dynamics due to its interplay between the low-energy barrier of the transition state and the evolution of the zero-point energy along the reaction path [5, 6]. Our study of reactions (3) was motivated by the opportunity to benchmark our results against a previously published merged-beams measurement, and we performed new calculations of the involved potential energy surfaces to understand the experimental results. And for reactions (4) we investigated the branching ratio of the two product channels, which is important for accurately modeling the gas-phase formation of water in the diffuse and dense molecular clouds.

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Energy and angular distributions in low-energy electron and argon atom collisions

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Study the electron impact ionization cross sections still has a great interest both experimenally and theoretically [1-2] due to their numerous applications.
In this work we present total, energy and angular differential cross sections for single-ionization in collision between electron and argon atom. We treat the collision problem classically using the three body approximation. The target atoms are described within the single active electron approximation using Garvey model potential where only the outermost electron is involved in the collision dynamics [3]. During our simulations the projectile energy was between 50 eV and 1 keV. Figure. 1 shows the energy differential cross total cross sections of the single electron ionization at 250 eV e^- − Ar (3p) collisions. We found that our present CTMC model describe reasonable well the ionisation cross sections and agree with our experimental data.

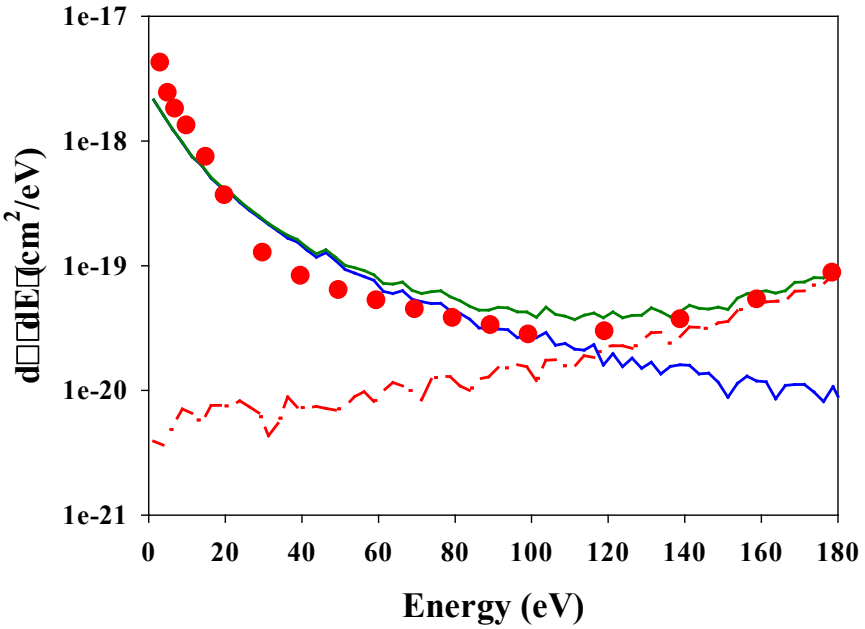

FIG. 1: Energy differential cross sections by 250 eV electron impact on argon target. Solid red circle: Experimental data, red dashed line: present CTMC results, projectile electron contribution, blue line: present CTMC results, target electron contribution, green line: present CTMC results, sum of the projectile and target electron contribution.

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Ionization and charge exchange cross sections in collisions between singly charged ions and ground-state atomic nitrogen

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Electron processes induced in ion-atom collisions are crucial and central in various research domains such as fusion plasma in tokamak reactors [1]. The modeling and control of these processes rely on the accurate cross sections of the induced electron processes.
In this work we present total single-ionization and single charge exchange cross sections in collision between singly charged ions and the ground-state atomic nitrogen. We treat the collision problem classically based on the three-body classical trajectory Monte Carlo model [2]. The nitrogen atom is described within the single active electron approximation using Garvey model potential where only the outermost electron is involved in the collision dynamics [3]. Regarding the projectile, in the first approximation, it is treated as a frozen core model and the charge of the projectiles are +1 in the entire time of the collision. In the second approximation, the projectile-target interaction is described by a model potential which takes into account the screening effect applied by the projectile electrons [3]. In Fig. 1, we present the total charge exchange cross sections at $Li^+ - N(2p)$ collisions. Our present CTMC results are in a good agreement with the experimental data of Pivovar et al. [4].

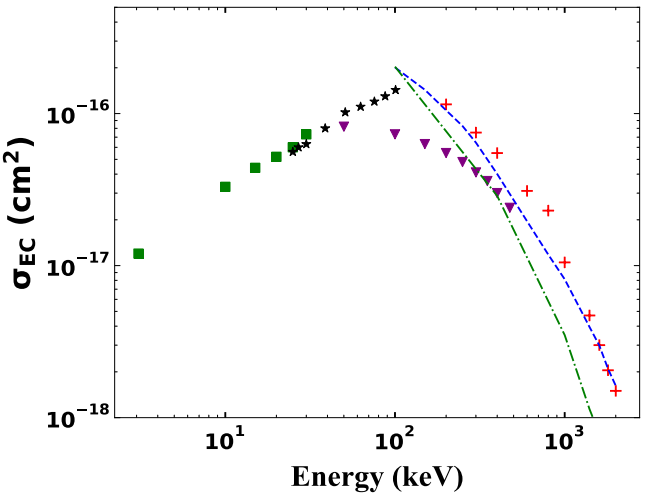

FIGURE 1. Total cross sections of the single-electron capture in $Li^+ - N(2p)$ collision system as a function of the projectile impact energy. - - - - CTMC results including projectile electrons screening effect and -·-·- frozen-core CTMC results. Experiments: + Pivovar et al. [4], ▼ Allison et al. [5], ■ Kikiani et al. [6] and ★Lockwood [7]

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Disentangling the relationship between S_N2 and E2 reactions in ethyl halides

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The bimolecular nucleophilic substitution reaction (S_N2) and bimolecular elimination reaction (E2) are two essential reaction types in organic chemistry [1]. As both reactions lead to the same ionic product, it is inherently difficult to distinguish between them solely with experimental approaches. In an attempt to overcome this experimental deficiency, we measured the reaction of fluoride with iodoethane and its fully β-carbon-fluorinated counterpart. The latter leads to the complete suppression of the E2 pathway. Here, we report the results of the reactions in the gas phase at four collision energies between 0.4 and 2 eV. For these measurements, we employed a crossed molecular beam setup combined with a velocity map imaging spectrometer. The obtained energy and angle differential cross-sections can reveal a mechanistic understanding of reaction dynamics on an atomic level [2], especially in cooperation with state-of-the-art theory [3]. In the reaction with CF_3CH_2I, we observe an increased signal in the proton transfer channel, which is negligible in the reaction with CH_3CH_2I. Furthermore, at higher collision energies, the formation of CF_2CI^- becomes the dominant channel, while no similar product is observed in the unfluorinated case. In Figure 1 the differential cross-sections for iodide stemming from the reaction of F^- with CH_3CH_2I and CF_3CH_2I are depicted. In the first case the product ions can stem from both the S_N2 and the E2 pathway while in the latter the source is solely S_N2.

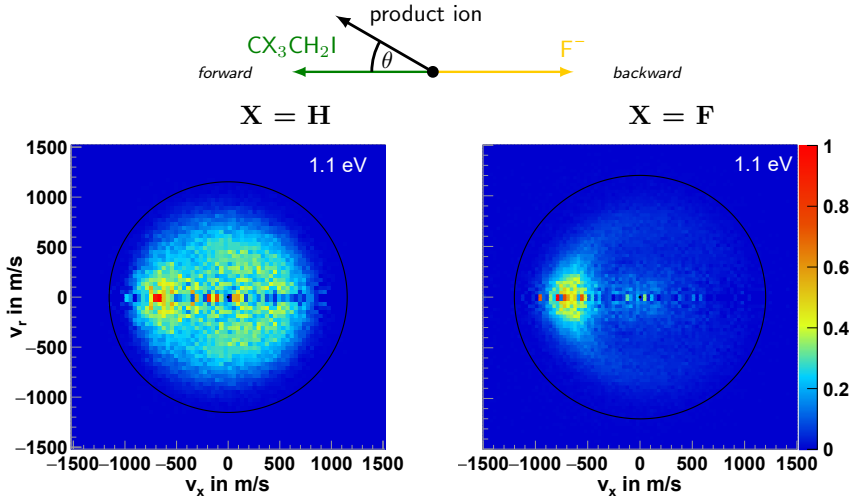

Figure 1: Three dimensional velocity distributions for I^- stemming from the reactions F^-+CH_3CH_2I (left panel) and F^-+CF_3CH_2I (right panel) in the center of mass frame.

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Multiphoton double ionization of H_2 induced by attosecond pulses

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Pump-probe experiments are nowadays able to unravel the role of nuclear motion and electron correlation in excitation and ionization processes in molecules on the ultrashort time scale. The interaction of intense short light pulses with molecular systems necessarily implies the solution of the time-dependent Schrodinger equation (TDSE) in a configuration space that comprises all break-up channels. The resolution of the TDSE in full dimensionality for two electrons targets, such as He or H_2, already represents a non-trivial task, but it is the only sensible approach to extract reliable information on the role of electron-electron and electron-nuclear correlation terms. For the hydrogen molecule, the main difficulty lies on the fact that, for solving the problem of molecular double ionization, it is mandatory to solve the four-body coulomb break-up to include all the possible paths and be able to extract the observables of the double ionization from the out-going wave packets. On this work, we have implemented a new computational tool allowing us to describe the four-body coulomb break-up accounting for both electronic and nuclear motions at equal footing, thus beyond the Born-Oppenheimer approximation. We employ a description of the wave function written in a basis set of FEM-DVR (finite element method combined with a discrete variable representation) [1,2]. We use an exterior complex scaling procedure to impose the appropriate many-body Coulomb boundary conditions in a defined volume [1,3,4]. We have first checked our implementation by comparing with existing theoretical data on one- and two-photon double ionization within the fixed nuclei approximation [5,6], and examine what is the role of nuclear motion, in particular, when the two-photon sequential double ionization path is energetically allowed.

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SESSON 2

Attosecond photoionization time delays in Acetylene

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Attosecond pump-probe spectroscopy techniques offer the possibility to track and control electron dynamics in matter. Among the different techniques available, the RABBITT technique (acronym for Reconstruction of Attosecond Beating By Interference of Two-photon transitions) has been employed to extract photoionization time delays in atoms, and more recently in molecules and solids. Initially conceived as a method for the temporal characterization of trains of attosecond pulses [1], this technique employs an attosecond XUV pulse train in combination with a weak IR field leading to an interferometric signal from which dynamical information on the photoelectron emission can be extracted with attosecond resolution. This information is encoded in the resulting photoelectron spectrum measured as a function of the time delay between the train and the IR field. The spectrum captures the so-called mainbands, resulting from a one-photon absorption induced by the XUV attosecond pulse train, along with the interferometric signal (sidebands) resulting from the absorption of an XUV photon and the absorption or emission of an IR photon. From this signal, it is possible to retrieve the photoionization time-delays. The most recent applications in molecules have shown that the vibrationally resolved RABBIT spectra of diatomic [2] and polyatomic [3] molecules further allows one to capture changes induced by the nuclear motion, as, e.g., on the centrifugal barrier seen by an escaping photoelectron.

We will present our most recent theoretical results applying the RABBITT technique to acetylene. We investigate an energy range where up to four valence-channels ($X^2\Pi_u$, $A^2\Sigma_g^+$, $B^2\Sigma_u^+$ and $C^2\Sigma_g^+$) are energetically open. We examine the photoelectron spectra and analyze the dependencies of the resulting photoionization time-delays with the molecular orientation with respect to the light polarization. In particular, following our previous work on CF4 [4], we show how the RABBITT spectra is significantly modified due to IR-induced transitions between the different cationic states. The theoretical methodology employed for this calculations consisted in solving the time-dependent Schödinger equation in a basis of Kohn-Sham orbitals and using the exclusive probability formalism to include interchannel couplings [4]. The basis is obtained in the dipole and static-exchange approximations by solving the Kohn-Shbam Hamiltonian using a B-spline multicenter approach and the LB94 functional [5]. All the calculations have been performed in the fixed nuclei approximation.

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High resolution molecular spectroscopy in micrometric thin cells

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Shrinking the size of atomic and molecular thin cells is a fascinating prospect with applications for quantum sensing and fundamental physics measurements. Miniature atomic cells were proposed for example as portable atomic clocks and hollow core fibers were filled with molecular gases for applications in frequency referencing [1]. Although compact, the confinement in the above devices remain mesoscopic (larger than the excitation wavelength). Atomic thin cells have been used to probe atoms under sub-wavelength confinement conditions allowing fundamental studies of the Dicke effect [2] and applications in quantum technologies [3]. High resolution probing of sub-wavelength confined molecules is more challenging, due to the small probabilities of molecular transitions, and was so far demonstrated only on a macroscopic cell via selective reflection spectroscopy [4]. Here we extend thin cell platforms to high-resolution molecular spectroscopy. We probe the $\nu 1+\nu 3$ line of acetylene at telecommunication wavelengths ($1.53\mu m$) and SF_6 as well as NH_3 rovibrations at mid-infrared wavelengths ($10.6\mu m$).

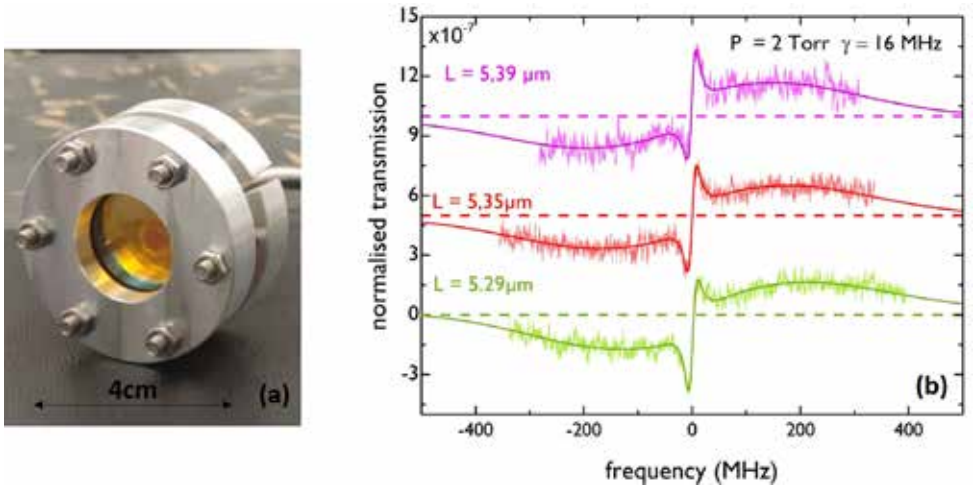

Figure 1: (a) thin cell photograph (b) transmission of an acetylene filled thin cell (2 Torr) at different thicknesses. Theoretical predictions [2] are shown as solid lines. The pressure broadening is 16MHz.

The thin cell was fabricated in our laboratory using ZnSe windows that are transparent through the near and mid infrared spectrum (Fig.1a). The thin cell thickness, measured by Fabry-Perot interferometry, is about $5.35\mu m$ with small variations of about $0.1\mu m$. This cell thickness corresponds to $\lambda/2$ for the SF_6 et NH_3 rovibrations and to $7\lambda/2$ for the combination line of acetylene, conditions for which a Dicke-type narrowing is expected [2]. In our experiments we detect the low power thin-cell optical transmission. A number of techniques were developed to increase the signal to noise ratio and remove the parasitic background from our signals [4]. Our experimental spectra, along with theoretical predictions are shown in Fig.1b. The excellent agreement between theory and experiments suggests that thin cell platforms are very well adapted for compact frequency referencing at telecommunication wavelengths and fundamental physics measurements.

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S2-P03

Electric-Quadrupole Isolated-Core Excitation of Sr below the $Sr^+(5g)$ Threshold

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The high lying doubly excited states of quasi-two-electron atoms, such as alkaline-earth-metal species, are ideal to investigate the dynamics of two highly excited electrons and study the quantum-mechanical three body problem. The efficient multiphoton excitation of high doubly excited states relies on the technique of isolated core excitation (ICE) [1]. In a first step, one of the two valence electrons is excited to a Rydberg state. The inner electron, residing in the ion core, is then excited in a sequence of resonant or nearly resonant transitions with energies close to those of the isolated ion. Such a scheme was for example used to excite planetary states of the Sr atom [2] and can be used for trapping [3] and nondestructively detecting [4] Rydberg atoms. In previous studies, ICE has been realized with electric-dipole core transitions. We report the observation of the ICE of Sr atoms with an *electric-quadrupole* transition corresponding to the excitation from the $Sr^+(5d_{5/2}$ to the $Sr^+(5g_{7/2,9/2})$ ion core states.

We experimentally and theoretically studied the photoexcitation spectra from $Sr(5d5/2nl)$ states ($n = 16 - 21, l = 12$), located high in energy in the Sr^+ continuum, to an energy region between the $Sr^+(5f)$ and $Sr^+(5g)$ ionization thresholds. They show series of lines attributed to $Sr(5gn''l'')$ states, which cannot be reached by electric-dipole ICE from $Sr(5d_{5/2}nl)$ states. We identified two competing mechanisms responsible for these lines: (i) the direct electric-quadrupole excitation from $Sr(5d_{5/2}nl)$ to $Sr(5gn'l)$ states, and (ii) the electric-dipole excitation to the weak $Sr(5fnl)$ component of the $Sr(5gn'l')$ states, this mixing being caused by the Coulomb interaction between the two excited electrons. The two excitation mechanisms can be unambiguously identified because they lead to spectra with different line-intensity distributions. A detailed analysis of the spectra is under way. ICE *via* nondipole core transitions opens new excitation pathways and will allow the excitation of doubly-excited states with, *e.g.*, larger angular momenta.

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S2-P04

Recent advances in the first principle simulation of attosecond XUV pump - XUV probe ionization spectra

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Recently, tunable sub-fs soft X-Ray (SXR) pulses became available at the LCLS X-Ray free electron laser (XFEL) at intensities that exceed those of current SXR high harmonic generation (HHG) sources by several orders of magnitude [1]. This overcomes the current intensity restriction of HHG based attosecond XUV pump-probe experiments to using XUV or SXR pulses as either the pump *or* the probe fields and thus paves the way for attosecond nonlinear X-Ray spectroscopic experiments that employ sub-fs SXR pulses for both pumping *and* probing ultrafast electron dynamics in molecules.

To identify these dynamics in transient spectra high level simulations covering (i) the ionization by the sub-fs SXR pump, (ii) the ensuing coupled electron-nuclear dynamics, and (iii) the interaction with the sub-fs SXR probe are desirable tools. However, each of the steps (i)-(iii) marks a formidable challenge already on its own. Their combination in a single study severely limits the tractable system size, in particular if the transient probe photoionization spectrum is sought after, which mandates an additional, more involved, ionization calculation for the probe step.

In this contribution we report an approach that marks a trade-off between computational cost and accuracy to facilitate the complete treatment (i)-(iii) in simulating sub-fs pump-probe photoionization spectra from XUV to SXR photon energies for small organic molecules. To this end, we employ complete active space wave functions with perturbative correlation energy correction (CASPT2) to describe the molecular bound states of the neutral, cationic and dicationic species, respectively. Further, the pump and probe ionization amplitudes are evaluated by a Dyson orbital approach, where the continuum states of the outgoing electron are obtained with the static exchange B-spline DFT method based on respective CASPT2 densities. Finally, the coupled electron-nuclear dynamics between the pump and probe interactions is modeled with the fewest switches trajectory surface hopping method, where an ensemble of trajectories represents the nuclear zero point energy spread.

The performance of the outlined protocol will be scrutinized for different molecules and various spectroscopic setups. Facilitating sub-fs XUV and SXR pulses, the dynamics induced by the pump ionization of valence orbitals are interrogated by probing either valence ionization, or core ionization, respectively. In addition to that we are going to study the performance of further simplifications to the outlined protocol, such as neglecting the motion of the nuclei and disregarding the explicit evaluation of the continuum states for the probe ionization step, i.e., the sudden approximation.

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Resonant Perfect Absorption Revealed by Attosecond Transient Absorption Spectroscopy in a Macroscopic Medium

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We propose and study the manipulation of the macroscopic transient absorption of an open two-level system via temporal engineering. By imposing a femtosecond temporal gate on the polarization decay, we confine the free evolution of the system and therefore the natural reshaping of the excitation pulse in a macroscopic medium. As demonstrated by numerical and analytical simulations, the resonant absorption of light can be reduced or significantly enhanced by employing an intense laser field relative to the laser-free case. A particular finding is the achievement of the near-complete extinction of light at the resonant frequency, which may be regarded as resonant perfect absorption. This spectral feature arises from the full destructive interference between the excitation pulse and its subpulses developed and tailored during propagation, and is further revealed to be connected with the formation of zero-area pulses in the time domain. The presented scheme is formally similar to the time-gating approach employed for addressing the ultrafast buildup of absorption profiles [1,2], while the observed phenomenon is reminiscent of the investigations of coherent perfect absorbers devised [3] and realized [4] a decade ago. We expect a synergic combination of precise temporal control and spectral phase manipulation in macroscopic media to open new routes for the control of high-frequency light and its interaction with matter.

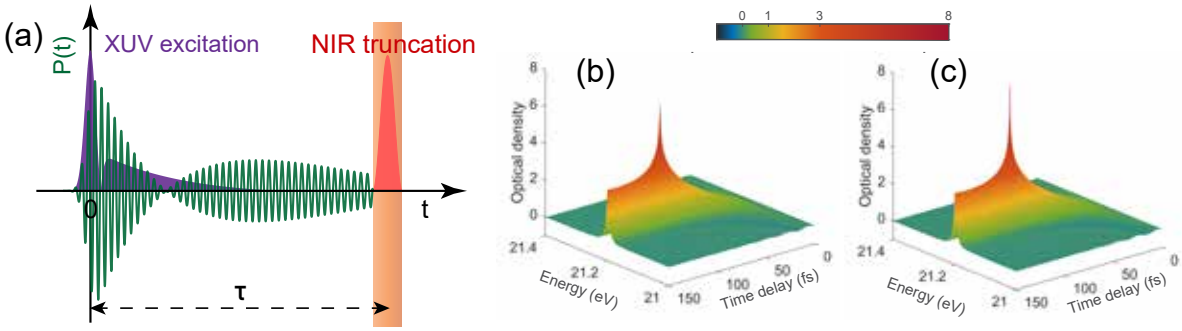

FIG. 1: (a) Schematic illustration of laser-gated resonance in a macroscopic medium: the polarization response (green) triggered by the extreme-ultraviolet (XUV) pulse evolves and is then truncated by a time-delayed near-infrared (NIR) pulse. The excitation XUV will get reshaped and develop a tail when propagation effects are included. (b) Numerical and (c) analytical transient absorption spectra in the vicinity of the transition frequency.

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One- and two-axis squeezing via laser coupling in an atomic Fermi-Hubbard model

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We study the Ramsey-type spectroscopy and the production of spin-squeezed states with ultra-cold atomic fermions described by the Fermi-Hubbard model in the Mott insulating regime. We show activation of two twisting mechanisms by a position-dependent laser coupling between internal degrees of freedom of atoms. A single laser coupling simulates the one-axis twisting model with the axis and direction of squeezing determined by the value of phase defining the atom-laser coupling. As such, adding a second laser beam with an adequately chosen phase paves the way to simulate the two-axis counter-twisting model, allowing reaching the Heisenberg-limited level of squeezing. The scheme can be implemented readily in state-of-the-art optical lattice clocks.

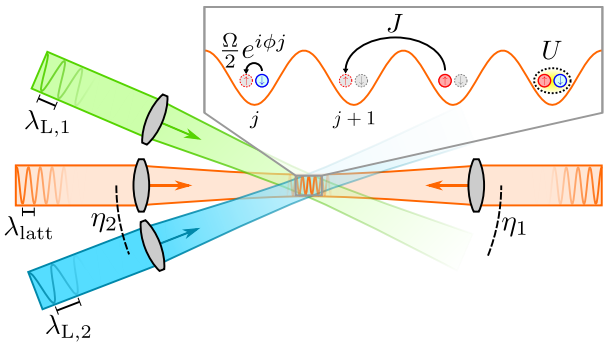

FIG. 1: Fermi-Hubbard model (FHM) for atoms in optical lattices or tweezer arrays with nearest-neighbor tunneling rate J, on-site interaction U and additional coupling between atomic internal degrees of freedom with position-dependent strength $\Omega e^{i\phi j}$. The coupling can be realized with one or two off-resonant laser beams.

Progress towards a measurement of the electron electric dipole moment with YbF molecules

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The search for the electric dipole moment of the electron (eEDM) is one of the most stringent tests for CP-violating physics beyond the Standard Model. The current upper limit, $|d_e| < 1.1 \times 10^{-29}$ e cm, constrains new CP-violating physics to energy scales above 3 TeV [1]. The most sensitive searches for the eEDM use heavy polar molecules, such as YbF [2], HfF^+ [3] and ThO [1].

We report on a series of new techniques that have improved the statistical sensitivity of the YbF eEDM experiment [4]. We have increased the number of molecules participating in the experiment by an order of magnitude using a carefully designed optical pumping scheme. We have also increased the detection efficiency of these molecules by another order of magnitude using an optical cycling scheme. In addition, we show how to destabilise dark states and reduce backgrounds that otherwise limit the efficiency of these techniques. Together, these improvements allow us to demonstrate a statistical sensitivity of 1.8×10^{-28} e cm after one day of measurement, which is 1.2 times the shot-noise limit. We will also discuss ongoing investigations of systematic errors on the experiment. The current level of sensitivity will allow us to measure the eEDM at the 10^{-29} e cm level with 100 days of data.

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Dissociative Photoionization of EUV Lithography Photoresist Models

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The dissociative photoionization of model molecules for extreme ultraviolet (EUV) lithography photoresists used in the production of integrated circuits was investigated to get mechanistic insights that are important for improving photoresists materials and developing better electronic devices. The semiconductor industry has recently adopted EUV lithography (13.5 nm, 92 eV) to enable printing sub-10 nm features on wafers. However, stochastic print failures are often decreasing the yield in the manufacturing process. The origins of these defects are not definitively clear since little is known about the chemical mechanism in EUV photoresist materials that is induced by interaction with EUV light. As those materials are complex compositions and the complete reaction mechanism involves photoionization, radiation chemistry by secondary electrons and diffusion in the thin film, these sub-steps need to be disentangled and investigated independently. We studied the interaction of photoresist prototype compounds using EUV synchrotron radiation and employing photoelectron spectroscopy and photoelectron-photoion coincidence (PEPICO) detection at the GasPhase beamline at Elettra Sincrotrone Trieste [1].

Tert-butyl methylmethacrylate is a monomer unit widely used in the common ESCAP (environmentally stable chemically amplified photoresist) resist class [2], in which the interaction with light induces an acid-catalyzed transformation. This leads to a solubility switch enabling the pattern formation after development. The PEPICO experiments on *tert*-butyl methylmethacrylate show that interaction with 92 EUV photons almost always leads to dissociative photoionization into various channels depending on the binding energy. Interestingly, the experiment and quantum chemical computations reveal that dissociative photoionization can also lead directly to the desired ester hydrolysis. Here, the parent ion undergoes a McLafferty rearrangement and dissociates into the isobutene cation and neutral methacrylic acid.

These gas phase experiments complement parallel research on thin films conducted at imec using time-averaged and time-resolved spectroscopic techniques. First of all, however, they give unique insights into the initial step in EUV lithography, photoionization, for a better understanding of the mechanism, necessary to make EUV lithography more profitable.

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Trapping Ions and Ion Coulomb Crystals in a 1D Optical Lattice

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Optically trapped ion Coulomb crystals are an interesting platform for quantum simulations due to the long range of the Coulomb interaction between the ions as well as the state dependence of the optical potential allowing the generation of versatile trapping geometries. Furthermore, micromotion is orders of magnitude lower in optical traps than in rf-traps. This could give optical traps an edge on rf-traps in applications in which micromotion limits the perfomance. This includes the study of atom-ion interactions at ultracold temperatures where this driven motion leads to a limit on the achievable interaction energies [1]. Additionally, they might offer a platform to study quantum structural phase transitions from 1D (linear) to 2D (zigzag) crystals in a controlled way [2,3], where micromotion inherently causes decoherence. Optical lattices extend this platform by providing an array of individual microtraps for the ions. This expands the possible applications of the system to study friction and oscillator-chain models [4-6]. As optical lattices are extendable in size and dimension they might allow the realization of ion-microtrap structures in 2D and 3D.

In the past we reported the successful trapping of a single ion in a one-dimensional optical lattice [7] as well as of ion Coulomb crystals in a single beam optical dipole trap [8]. In this poster, we present recent advancements in trapping $^{138}Ba^{+}$ ions in a one-dimensional optical lattice at a wavelength of 532nm and the first successful trapping of small ion Coulomb crystals ($N \leq 3$). We compare the trapping performance of different configurations of the optical dipole trap to demonstrate a gain in the trap depth due to interference in the case of a lattice. We demonstrate single site confinement of the ions in the lattice by showing reduced displacement by axial electrostatic fields and increased motional frequencies compared to a trap where beams of orthogonal polarization are overlapped.

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Transition intensities of trivalent lanthanide ions in solids: Extending the Judd-Ofelt theory

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The Judd-Ofelt (JO) theory has been successfully applied since almost 60 years [1, 2], to interpret the intensities of absorption and emission lines of crystals and glasses doped with trivalent lanthanide ions (Ln^{3+}). Despite its remarkable efficiency, this standard JO theory cannot reproduce some of the observed transitions, because of its strong selection rules. It is especially the case for europium (Eu^{3+}), well known to challenge the standard JO theory [3, 4].

In this work, we present a modified version of the JO theory. In our model, the properties of the dopant are calculated with well-established atomic-structure techniques, while the influence of the crystal-field potential is described by three adjustable parameters. By applying our model to europium (Eu^{3+}) we are able to give a physical insight into all the transitions within the ground electronic configuration, and also to reproduce quantitatively experimental absorption oscillator strengths (see Fig. 1). Our model opens the possibility to interpret polarized-light transitions between individual levels of the ion-crystal system [7].

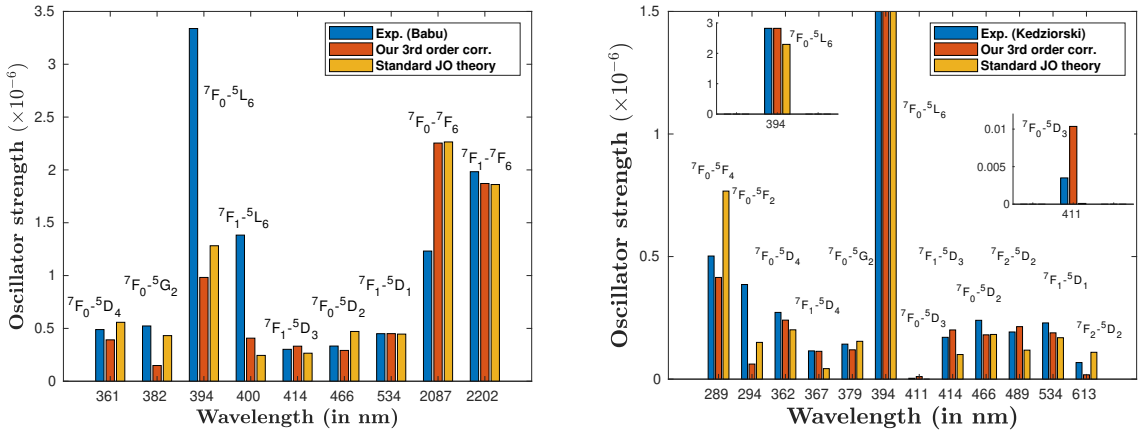

Figure 1: Comparison between experimental [5, 6] and theoretical oscillator strengths of absorption, plotted as function of the transition wavelength (not at scale). The transitions are labeled with the LS-term quantum numbers of the Eu^{3+} free ion.

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Improving the spectroscopic knowledge of neutral Neodymium

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Laser cooling has found wide application in science and technology. The success of laser cooling and trapping of lanthanides makes it possible to carry out new experiments with ultracold dipolar gases, for example for quantum simulation of solid state physics [1]. All quantities critical for such experiments are based on atomic energies and transition dipole moments (TDMs). Thus, the success of future ultracold experiments with new species is based on a detailed knowledge of their spectroscopy. For this purpose we use the semi-empirical method of atomic structure calculations based on the Cowan suite of codes [2, 3], to calculate the energy spectrum of neodymium (Nd). Particular attention is paid to accurately describing configuration-interaction (CI) mixing, to which TDMs are very sensitive. Since it belongs to the left side of the lanthanide series, Nd presents a dense spectrum in the range of 8000-15000 cm^{-1}, in striking contrast with atoms like dysprosium or erbium (see Fig. 1). This makes it challenging to identify the levels, especially for levels of $J = 4$, 5 and 6.

The calculations were carried out for three even parity configurations: $4f^4\ 6s^2$, $4f^4\ 5d\ 6s$, $4f^3\ 5d\ 6s\ 6p$, and three odd parity configurations: $4f^4\ 6s\ 6p$, $4f^3\ 5d\ 6s^2$ and $4f^3\ 5d^2\ 6s$. For the least square fitting, we use values from the NIST database as reference energy levels [4]. The primary source of data on neutral Nd levels in the database is Martin *et al.* [5]. For even parity, 83 levels were included, 25 of which were not interpreted in the NIST database. The energy levels range from 10000 cm^{-1} to 29000 cm^{-1}. There are 12 parameters in the fit. After the calculations the standard deviation is 90 cm^{-1}. For odd parity, we have included 221 levels. 124 levels were not interpreted in NIST. There are 15 parameters in the fit. Standard deviation for this parity is 85 cm^{-1}, while the energy levels range from 6000 cm^{-1} to 29000 cm^{-1}.

Through this careful spectroscopic calculation, we have improved the spectroscopic knowledge of Nd. The next step will be to calculate the TDMs and Einstein coefficients, which are necessary to characterize the efficiency of laser cooling and trapping of atoms.

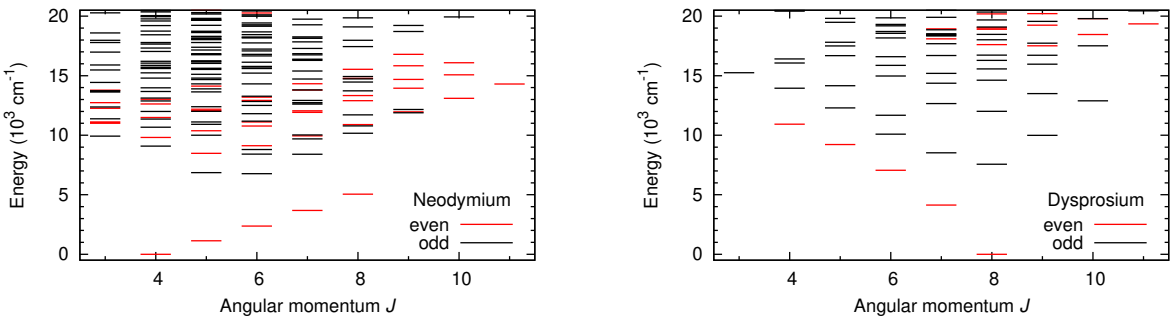

Figure 1: Energy diagrams as functions of the electronic angular momentum J and sorted by electronic parity are shown for neodymium (Nd, left panel) and dysprosium (Dy, right panel).

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Quantum phases of bosonic chiral molecules in helicity lattices

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Chiral molecules have attracted significant multidisciplinary attention for many decades, from pharmaceuticals and the life sciences to quantum chemistry and optics. Of particular importance is the ability to identify and separate molecules of different chirality (known as enantiomers of each other), a process usually referred to as chiral discrimination [1].

Recently, the progress on laser cooling has opened the possibility of cooling chiral molecules to the ultracold regime in the following years [2, 3]. This will possibly open exciting new directions in the study of chiral molecules, much in analogy to the already well-established cold atom gases.

Anticipating these developments, in this work we theoretically study the phase diagram of cold and interacting chiral molecules immersed in recently proposed *helicity lattices* [4]. The lattices have homogeneous mean squared values of the electric field, but spatially varying helicity, and thus, they exert a discriminatory force on chiral molecules with different handedness [5]. We model these lattices with an extended Bose-Hubbard model [6], where the chiral molecules are represented as structureless bosonic particles which interact through repulsive on-site and dipolar long-range interactions.

We provide a detailed presentation of the different quantum phases shown by the helicity lattices. In particular, we find that a strong dipole-dipole repulsion between molecules results in the polarization of left/right enantiomers. In an experiment, this would produce a phase separation of enantiomers, acting as an alternative route towards chiral discrimination.

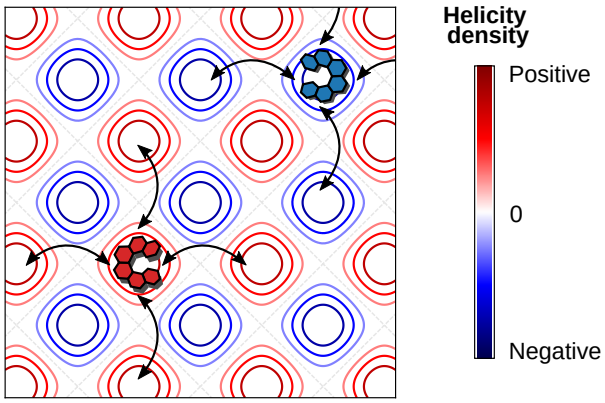

FIG. 1: Illustration of a square helicity lattice. Red and blue regions correspond to sites with opposite helicity densities. We assume that left (right) enantiomers can only move within red (blue) sites.

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Two Electron Processes in Relaxation of Hollow Atoms

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The M-X-rays emitted from Rydberg (n~30) hollow atoms (RHA) created in collisions of highly charged Xe^{q+} ions (q=23-36) with Be surface were measured and interpreted in terms of the MCDF calculations [1] as a cascade of nf-3d electric dipole X-ray transitions, including their M-shell hypersatellites. The measured X-ray spectra indicate the importance of two-electron processes, in particular the Internal Dielectronic Excitation (IDE) [2] and Two-Electron One-Photon (TEOP) transitions in relaxation of studied RHA. In fact, the observed M-X-rays for Xe^{26+} ions (see Fig. 1), that have no initial vacancies in 3d subshell, result from filling 3d vacancies formed exclusively by the IDE. We found a sharp cut-off for X-ray cascade at n~10-20, which supports the idea that for higher n-states the relaxation proceeds via the Interatomic Coulombic Decay (ICD) [3]. We demonstrate that present observations explain why the relaxation of RHA can proceed in the ultrafast timescale.

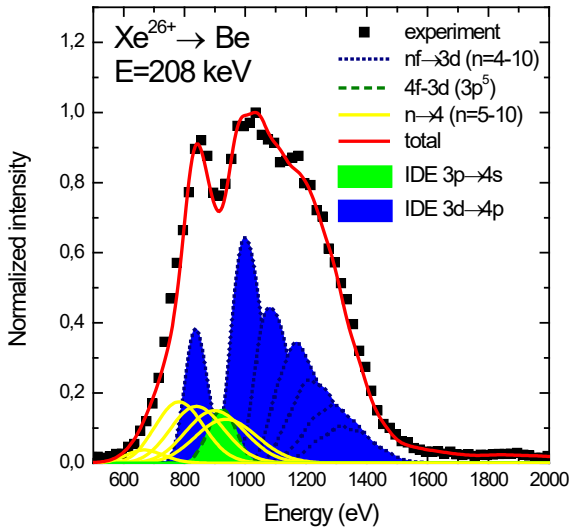

FIG. 1: Measured spectrum of X-rays for 208 keV Xe^{26+} ions colliding with Be foil interpreted as a cascade of nf-3d transitions to vacancies created exclusively by the IDE process.

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A high-resolution asymmetric von Hamos spectrometer for low-energy X-ray spectroscopy at the CRYRING@ESR electron cooler

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A high-resolution asymmetric von Hamos spectrometer for low-energy X-ray spectroscopy experiments at the electron cooler of CRYRING [1] in the international Facility for Antiproton and Ion Research (FAIR) in Darmstadt is presented. The spectrometer will allow to measure, with a high resolution of down to 100 meV, the low-energy X-rays (5-10 keV) from radiative recombination (RR) of stored bare or few-electron mid-Z ions interacting with cooling electrons. For these ions the calculated one-loop Lamb shift is about 2-5 eV, being much larger than the nuclear size effect contributing about 15-120 meV [2]. Performed Monte-Carlo X-ray tracing simulations [3] show that the high resolution of the spectrometer will give access to study the QED effects in mid-Z H-like ions with a high precision.

The proposed asymmetric von Hamos spectrometer benefits from the unique features of RR X-ray emission in the electron cooler of CRYRING@ESR, the extremely long-linear ($\sim$ 1 m $\times$ 1 mm) X-ray source accepted by von Hamos geometry and very cold electron beam temperature of about meV. In order to control the Doppler effect, two copies of the asymmetric von Hamos spectrometer will be installed next to the dipole magnets on both sides of the electron cooler and to detect blue (0°) and red (180°) shifted RR X-rays, what allows to eliminate completely the influence of Doppler effect on measured X-ray energies.

The dispersive plane of the asymmetric von Hamos spectrometers will be oriented horizontally. Both the diffraction crystal and the X-ray detector will be mounted on the 4-axis motorized goniometers to secure the adjustment of their position for various bending radii of the crystal. The stepping precision of the linear and rotational movements will be 1 μm and 0.001°, respectively, which enables the necessary fine tuning of the positions and angles of the crystal and X-ray detector. Both spectrometers will be equipped with a Si(111) crystals, cylindrically bent to radius of 1 m. The diffracted X-rays will be measured by the position-sensitive Timepix3 detector that is sensitive to the hitting position (256 $\times$ 256 pixels with size of 55 $\times$ 55 μm^2) and time (1.6 ns resolution) of the registered photon. The spectrometers will be mounted on-cooler-axis to the dedicated intermediate vacuum chambers.

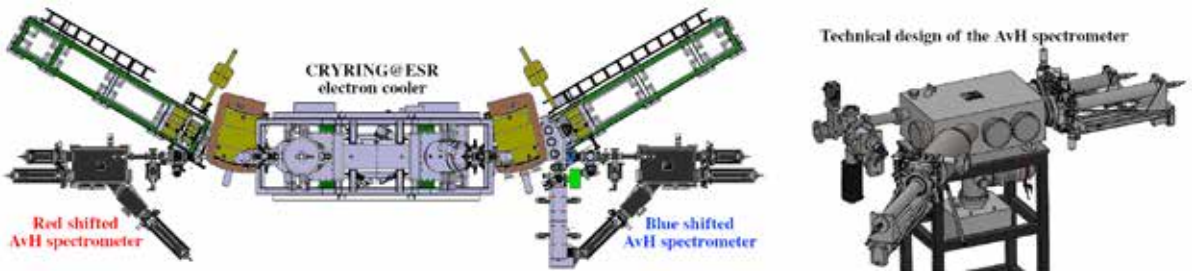

FIG. 1:Technical drawing of the AvH spectrometers installed at CRYRING@ESR electron cooler.

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Modeling Molecular Aggregates Using Dirac-Frenkel Variational Method

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The linear absorption spectrum of H and J molecular aggregates, where both the electronic and vibrational molecular degrees of freedom are considered. It is made up of a collection of molecules (*sites*) coupled via an electrostatic dipole-dipole interaction. Intramolecular vibrational modes are modeled as harmonic oscillators. Molecular aggregate excitation dynamics and spectra can be computed using the wavefunction based time-dependent Dirac-Frenkel variational principle by postulating an Ansatz wavefunction, which ought to be complex enough to represent all the necesary electron-vibrational quantum states of the aggregate.

Vibronic states can be represented using the multi-Davydov D_2 (mD_2) Ansatz [1], given by

$$|\Psi_{mD_2}(t)\rangle = \sum_m^M \sum_n \alpha_{i,n}(t)\,|n\rangle \otimes |\boldsymbol{\lambda}_m(t)\rangle, \tag{1}$$

where $|n\rangle = |1_n\rangle \bigotimes_{m\neq n} |0_m\rangle$ is an electronic state with amplitude $\alpha_n(t)$, which define a singly excited nth site. Intramolecular vibrational mode state is represented in terms of the multidimensional time-dependent coherent states $|\boldsymbol{\lambda}_m(t)\rangle = \bigotimes_{k,q} |\lambda_{m,kq}(t)\rangle$, where $|\lambda_{m,kq}(t)\rangle$ is an mth coherent state multiple of a qth mode coupled to the kth site. By consider a sufficient number of multiples M, Dirac-Frenkel variational method with mD_2 Ansatz can match accuracy of the Hierarchical Equations of Motion and Multi-Configuration Time-Dependent Hartree methods [2].

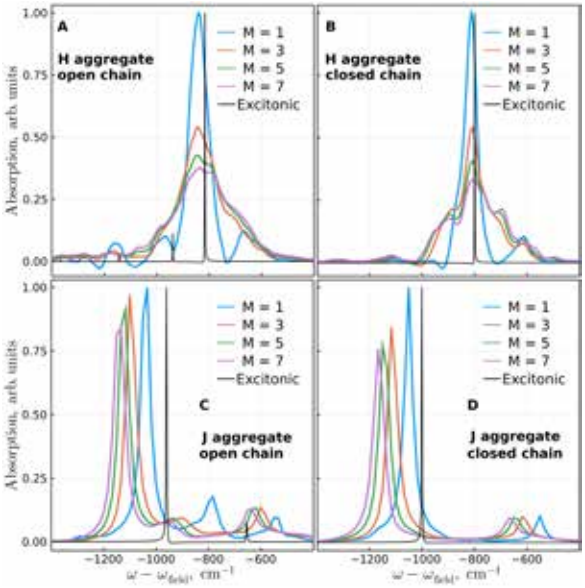

Fig. 1. Absorption spectrum of the model H aggregate in (A) chain and (B) ring configuration, computed with an increasing number of Davydov D_2 multiples M considered. Purely excitonic spectrum is also shown.

By inspecting and comparing absorption spectra of both the ring and chain aggregates over a range of electrostatic nearest neighbor coupling and temperature values, we find the mD_2 Ansatz with multiplicity of $M = 7$ is required to obtain accurate aggregate absorption spectrum, while the regular D_2 Ansatz (Eq. (1) with $M = 1$) is not sufficient. For H aggregates, see Fig. (1), multiplicity is required to obtain absorption lineshape positivity and correct peak intensities. For J aggregates, increasing the number of multiples considered, mostly just redshifts whole absorption spectrum, keeping the overall lineshape qualitatively the same, especially in ring aggregate. Due to vibronic energy level structure of an aggregate, vibrational mode coordinate and momentum variances exhibit out-of-phase oscillatory behaviour and an overall wavepacket broadening, which again is not captured by the non-multiple D_2 Ansatz.

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Neutral Atoms in Tweezer Arrays for Hybrid Quantum Computing

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Our project has the goal of building a quantum co-processor consisting of neutral atoms in tweezer arrays. This quantum co-processor will form part of an online-accessible hybrid quantum computer tailored for solving quantum chemistry problems.

The quantum co-processor will consist of strontium-88 atoms trapped in 2-dimensional arrays of optical tweezers, with a single atom trapped per tweezer. Qubit states will be encoded on the $^1S_0$ and $^3P_0$ electronic states of the atoms. Laser driven site selective single qubit rotations will be performed on the doubly dipole forbidden $^1S_0 \leftrightarrow {}^3P_0$ optical clock transition. Global excitations to Rydberg states will be used to generate entanglement between the qubits.

We report on our progress in the development of the 2nd generation strontium-based system in Eindhoven (see FIG 1), whilst the existing 1st generation system is situated in Amsterdam. We also report on the status of our rubidium-based system in Eindhoven (see FIG 2), which will be used to test various components before integration into the new strontium-based system.

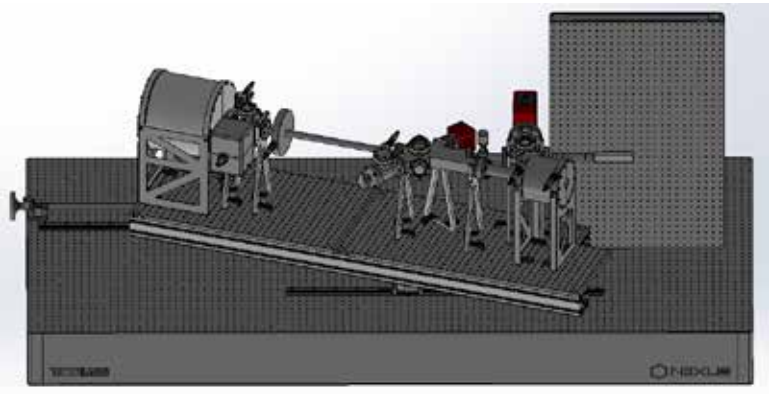

FIG. 1: CAD of vacuum system for the 2nd generation strontium-based system.

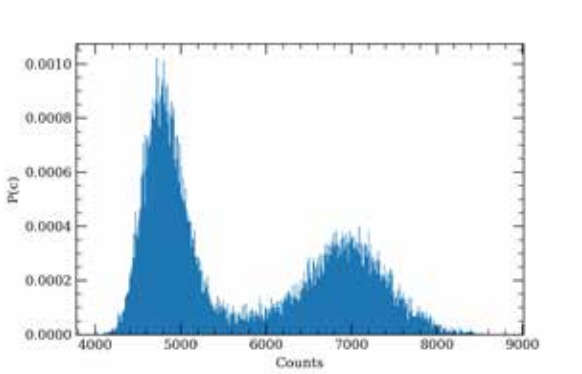

FIG. 2: Probability distribution of camera counts for repeated loading of a 3x3 tweezer array of single ^{85}Rb atoms with $\approx 50\%$ single atom probability per array site.

Using second order correlation to measure femtosecond impulses

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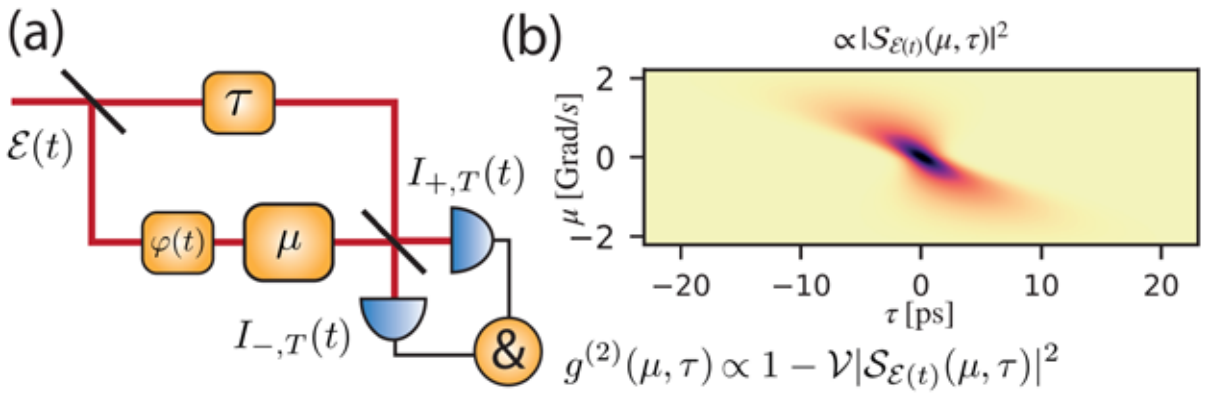
We examined the Hong-Ou-Mandel effect for coherent states of a femtosecond laser shifted in frequency and time domain. To achieve frequency shift we used an electrooptical phase modulator which required both a laser beam and RF signal synchronized with it. To callibrate our setup we used a custom ultra-resolution spectrometer based on a linear photodiode detector. We narrowed the laser's spectrum using a 4f setup with a precise slit. We are planning to modify our experiment by putting a special rubidium cell to the optical system and use photons from Sagnac interferometer which will ewentually allow us to obtain the phase matching function of the used PPKTP crystal.



(a) Ideational scheme - in the upper arm time shifting, in the bottom frequency shifting and phase modulation
(b) Expected shape of the second order correlation function with respect to time and frequency shifts

Measuring the Electron's Electric Dipole Moment Using Ultracold YbF Molecules

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The standard model predicts an extremely tiny value for the electron's electric dipole moment (eEDM, d_e), $d_e \sim 10^{-44}$ e cm. By contrast, theories beyond the standard model predict much larger values, typically $d_e \approx 10^{-31} - 10^{-24}$ e cm. To date, the current experimental upper limit is set at $d_e < 1.1 \times 10^{-29}$ e cm [1-4]. Further improvements in experimental precision are likely to discover new physics or rule out most of the parameter space of popular theories. The eEDM can be measured through the precession of the electron spin in an applied electric field. The precision is enhanced enormously when the electron is bound into a heavy polar molecule. The statistical precision depends on the spin precession time so a slow, ultracold beam of molecules has the potential to measure the eEDM to greater precision than the current limit.

We use a beam of ultracold YbF molecules produced by a cryogenic buffer gas source and then laser cooled to 100uK in the two transverse axes [5]. Such cooling yields a 300-fold increase in the brightness of the beam, and potentially a 10-fold increase in the spin-precession time, leading to a projected statistical uncertainty below 10^{-30} e cm [6]. However, magnetic field noise can severely limit the statistical sensitivity to d_e. We have developed and characterised a four-layer magnetic shield with internal shim coils and a shielding factor of 10^6 in order to reduce the background field, the gradients, and the noise to the required level. Here we present our progress to date, with focus on magnetic shielding and transverse laser cooling.

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Evaluation of radiative and Auger electron emission following K-shell vacancy creation in iodine

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Conventional treatment of cancer using radiotherapy has to deal with an undesirable impact on healthy tissues. Side effects of such treatment depend on the part of body being affected and the type of the radiotherapy. On the other hand, nanomedicine offers possibilities to enhance the local doses in tumor regions and non-invasively monitor the yield of the applied therapy. The targeted therapy seems to be a promising approach for cancer treatment [1], as the development of the targeted delivery systems aims to minimize the side effects and increase the effectiveness of the treatment.

The aim of the current work is to study radiative and Auger cascade following a creation of the K-shell vacancy in the iodine atom and provide accurate data of the radiative and Auger electron emissions that can be used further in the modeling of their impact on biological systems. Iodine is one of the widely used radionuclide with potential application in the targeted therapy. Theoretical multiple-photoionization cross sections were previously investigated for the K shell of the Fe atom [2] and Fe^{2+} ion [3].

Radiative and Auger cascade is investigated by considering transitions among subconfigurations. Radiative and Auger cascade is studied for the subconfigurations of the I^+ $1s\,5s^2 5p^5$ configuration. The study of the radiative and Auger cascade includes 13104 configurations: I^+ – 10, I^{2+} – 82, I^{3+} – 371, I^{4+} – 1240, I^{5+} – 1083, I^{6+} – 1632, I^{7+} – 1981, I^{8+} – 2056, I^{9+} – 1755, I^{10+} – 1158, I^{11+} – 786, I^{12+} – 465, I^{13+} – 261, I^{14+} – 132, I^{15+} – 43, I^{16+} – 49. This corresponds to the 392611 subconfigurations: I^+ – 31, I^{2+} – 481, I^{3+} – 3485, I^{4+} – 17730, I^{5+} – 15830, I^{6+}: 34239, I^{7+} – 56736, I^{8+} – 74494, I^{9+} – 73883, I^{10+} – 53142, I^{11+} – 34384, I^{12+} – 17030, I^{13+} – 7458, I^{14+} – 2667, I^{15+} – 509, I^{16+} – 513. Therefore, it leads to large scale calculations which include ∼4 millions electric dipole transitions and ∼22 millions Auger transitions.

The ion yield for the radiative and Auger cascade following the K-shell decay in the I^+ ion is shown in Fig. 1. The states of the I^{6+} ion accumulate main population in the cascade process.The largest ionization stage reached in the study of the cascade is I^{16+}. Final populations of radiative and Auger cascade are lower than 1% for the I^+, I^{2+}, I^{3+}, I^{14+}, I^{15+}, and I^{16+} ions. The ground configurations of the I^+ – I^{5+} and I^{11+} – I^{16+} ions are mainly populated in the cascade process.

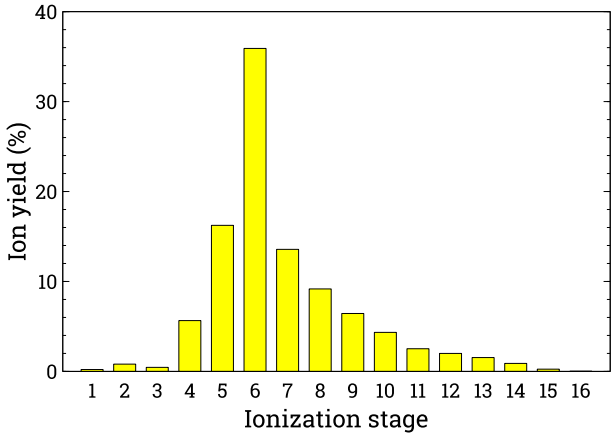

FIG. 1: The ion yields for radiative and Auger cascades following decay of the I^+ $1s\,5p^5$ configuration.

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Collisions between laser cooled molecules and atoms

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The formation and control of ultracold molecules is advancing rapidly, motivated by a broad range of exciting applications [1] including tests of fundamental physics, quantum information processing, and quantum chemistry. Collisions are crucial to this field and are a rich source of information about the interactions and reactions of atoms and molecules. Their control is important for evading losses and controlling reactivity [2], and they can be harnessed for sympathetic or evaporative cooling [3, 4].

Ultracold atom-molecule collisions have been investigated extensively by theory, but there are very few experimental studies. We present a summary of our work on inelastic collisions between CaF molecules and Rb atoms, in both a magneto-optical [5] and magnetic quadrupole [6] traps. In both traps we measure an atom induced loss rate of molecules close to the universal rate. In the magnetic trap, with the molecular sample prepared in the ground rotational state, we observe a 10-fold suppression in the loss rate, compared to the observed rate with molecules in the first excited rotational level. These observations are encouraging for the prospects of sympathetic cooling.

In addition, we will present our recent progress on experiments to confine the atom-molecule mixture in an optical trap and study collisions there.

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Effect of Vanadium implantation on the structure of glassy carbon

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Based on its unique properties of the carbon type materials, in this work we focus on the characterization of the glassy carbon and Vanadium implanted glassy carbon. Glassy carbon (GC) substrates were implanted with 25 keV Vanadium ions to a fluence ranging from 1 x 10^{12} to 1 x 10^{15} V^+/cm at room temperature. Raman spectroscopy was used to monitor the structural changes in the samples as a result of the implantation. The Raman spectrum of the pristine glassy carbon sample shows the characteristic D and G peaks at 1350 cm^{-1} and 1588 cm^{-1} [1]. Raman spectra of samples implanted at 1 x 10^{12}, 5 x 10^{12} and 1 x 10^{13} V^+/cm respectively show that the glassy carbon structure remain unchanged when compared to that of the pristine glassy carbon. This indicates that the low fluence implantation of Vanadium does not result in the radiation damage of the glassy carbon structure. High fluence implantation at 1 x 10^{14} and 1 x 10^{15} V^+/cm resulted in a slight change of the Raman spectrum of glassy carbon. The D and G peaks merged slightly into each other and became wider suggesting that the samples became damaged after implanting at these high fluence.

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Electron-Ion Recombination of N_2^+ Ions in Ground Vibrational State

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N_2^+ is one of the main ions in ionosphere of planets and moons such as Earth or Titan. Experimentally obtained data are not very consistent, as they differ by a factor of 2-3. The theory [Little et al] suggests, the problem is in the different rates of recombination for different vibrational states, which seems to be the main reason for the inconsistency. In different experiments were different vibrational populations [Sheehan et al].

We have performed measurements of recombination coefficient of N_2^+ ions with electrons using stationary afterglow apparatus with Cavity Ring-Down Spectroscopy and microwave diagnostics in temperature scale 150-250 K. We probed in situ the number densities of both ground and the first excited vibrational states of N_2^+. The population of the higher state is around 2%, therefore our data are appropriate for the ground vibrational state.

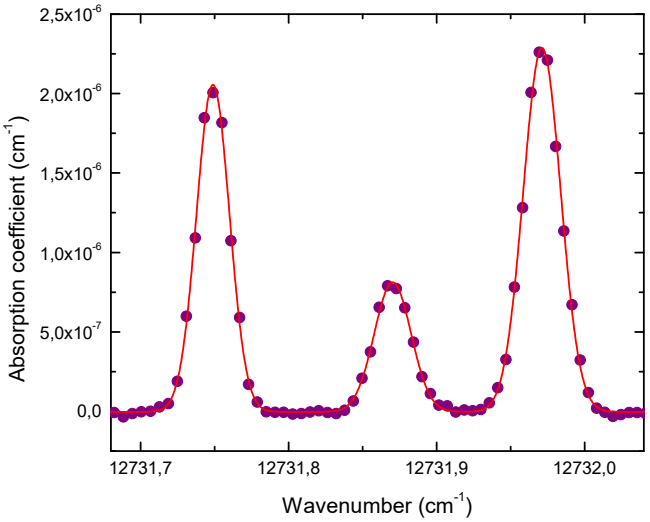

FIG. 1: Example of measured absorption line measured by Cavity Ring-Down Spectroscopy

Acknowledgement

This work was partly supported by the Czech Science Foundation (GACR 20-22000S & 22-05935S) and by the Charles University (project Nr. GAUK 337821).

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Two color all X-ray pump-probe spectroscopy of rotational dynamics

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In the present paper [**1**] we theoretically study the molecular rotation induced by X-ray photoionization using two-color all X-ray pump–probe spectroscopy. Upon ejection of a fast photoelectron by the first pump pulse, a molecule gains a recoil momentum, which not only kicks the molecule in the opposite direction, but may also induce its rotation around the center of mass. Although the photoelectron recoil effect does not create unidirectional rotation, we show that the angular recoil induces a recurrent modulation of the probe X-ray absorption signal as a function of the delay time between the two X-ray pulses. Contrary to the modern stationary X-ray spectroscopy, which is unable to resolve rotational structure, the proposed scheme allows for a real-time monitoring of the rotational dynamics with picosecond resolution. Schematic representation of the proposed two color X-ray pump-probe spectroscopy, which opens new perspectives in studies of molecular rotational dynamics induced by the recoil effect in real-time are given in Figure 1 and its caption.

We developed an accurate theory of the X-ray pump-probe spectroscopy of the recoil-induced rotation and study how the energy of the photoelectron and thermal dephasing affect the structure of the time-dependent X-ray absorption using the CO molecule as a case-study. We also discuss the feasibility of experimental observation of our theoretical findings, opening new perspectives in studies of molecular rotational dynamics.

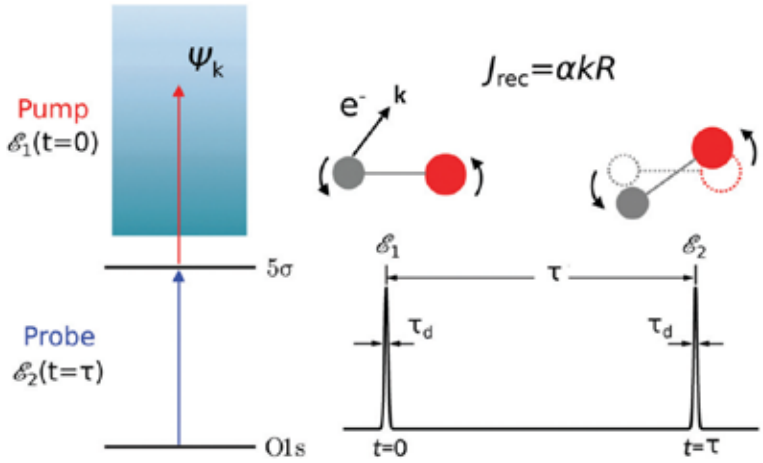

FIG. 1: Scheme of the electronic transitions (left panel) in the studied pump–probe process with two time delayed X-ray pulses (right panel). The pump X-ray pulse $\mathcal{E}_1$ (red arrow) at the instant $t = 0$ ionizes the electron from the HOMO 5σ to the continuum state $\psi_{\mathbf{k}}$. The ejected photoelectron with the momentum $\mathbf{k}$ transfers to the molecule recoil-induced angular momentum $J_{REC} = \alpha\mathbf{R} \times \mathbf{k}$ ($J_{REC} = J_{rec} \sin\theta$). Then, the time delayed probe X-ray pulse $\mathcal{E}_2$ (blue arrow) at time $t = \tau$ promotes the core electron of the oxygen atom O1s to the previously created valence hole in HOMO $\psi_{5\sigma}$ and probes the recoil-induced rotational dynamics.

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Special Issue "Ultrafast X-ray spectroscopy" of Molecules journal calls for contributions

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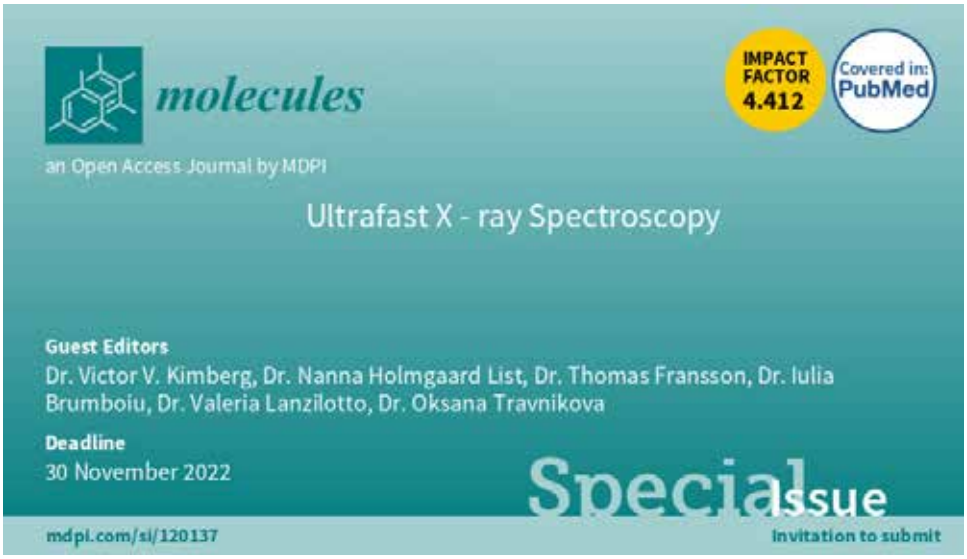
We invite you to submit an article for the Special Issue of Molecules, titled "Ultrafast X-ray spectroscopy". The recent development of a new generation of X-ray radiation sources and the great improvement in time and spectral resolution of experimental instruments can open up new qualitative possibilities for studying nature in unprecedented detail, with sub-femtosecond and sub- nanometer precision. Ultrafast photoinduced electronic and nuclear dynamics, which can be uncovered with the help of X-ray spectroscopy, lies in the basics of chemical reaction control, advances of material science and technology, as well as fundamental understanding of non-linear light–matter interaction.

This Special Issue invites contributions of recent advanced theoretical and experimental studies of various ultrafast processes (electronic, nuclear, or structural dynamics) in different systems ranging from single molecules to molecular clusters, molecular liquids, and condensed matter using X-rays as the main tool.

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in Molecules span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinar y topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.



S2-P25

Azimuthal Modulation of Electromagnetically Induced Grating using Structured Light

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When a strong coupling field in an Electromagnetically Induced Transparency (EIT)[1] scheme is replaced by a standing-wave (SW), Electromagnetically Induced Grating (EIG) is observed. Due to the spatial periodic modulation for the absorption and dispersion of the medium, implemented by the SW field, the traveling-wave (TW) probe field can be diffracted into higher order directions. EIG was widely investigated in different media[2,3] and has been extended to two-dimensions in multi-level atomic systems[4], involving non-linear modulation, as well as Raman processes[5].

On the other hand, a number of interesting effects arise when atoms interact with optical vortex beams, e.g. light beams carrying Orbital Angular Momentum (OAM). The OAM of light provides an additional degree of freedom in manipulation of optical information during the storage and retrieval of slow light[6], leading to novel applications in optical technologies such as data transmission, optical communication[7], optical tweezers[8], and quantum information[9].

In our work[10], we propose a theoretical scheme for creating a two-dimensional EIG in a three-level L-type atomic system interacting with a weak probe field and two simultaneous position-dependent coupling fields-a two dimensional SW and an optical vortex beam. We show that due to the azimuthal modulation of the optical vortex, a two-dimensional asymmetric grating is observed, giving an increase of the zeroth and high orders of diffraction, thus transferring the probe energy to the high orders of direction. The asymmetry is especially pronounced in the case of a resonant probe field and off-resonant SW and optical vortex fields. By analyzing the behavior of the different orders of diffraction for different values of the azimuthal number of the optical vortex beam, we explore the possibilities for direct control of the proposed EIG. Compared to other schemes, this grating is easily controlled by only adjusting the OAM number of the optical vortex field. By controlling the OAM number we can achieve a complete blocking of the diffracted photons at negative or positive angles, due to the interference effects between the amplitude and phase modulations of the system. Our findings are relevant for design of new quantum devices such as all-optical quantum switches and logic gates, as well as improving the performance of other EIT-based devices. This may find applications in all-optical information processing and atom-manipulation technologies. The experimental confirmation of the asymmetrical two-dimensional grating proposed here should be easily realized similarly to other EIG experiments in atomic media.

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Fano-ADC(2,2) Method for Multi-Electron Decay Processes

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Two-electron relaxation processes following inner-shell ionization of matter, such as the Auger effect or interatomic Coulombic decay, are known to play an important role in biological damage inflicted by radiation. Relevant mechanisms comprise acceleration of the photodissociation dynamics or the production of reactive secondary particles. Recent experiments suggest that even higher-order relaxation processes involving multi-electron transitions might reach surprisingly high intensities, both in molecules and in weakly bound clusters [1,2]. These hitherto little investigated mechanisms thus might also significantly affect the response of matter to radiation.

Among the fundamental characteristics of a metastable state belongs the decay width, directly related to its lifetime. One of the most successful approaches to *ab initio* computation of intra- and inter-atomic electronic decay widths, which has been utilized in several important studies of ICD [3] or collective decay processes involving more than two electrons [4], is the Fano-ADC method [5]. It is based on the Fano theory of resonances and algebraic diagrammatic construction in the intermediate state representation (ISR-ADC) [6] for the description of the many-electron wave function. Thus far, all implementations of the method were based on the extended second-order ADC scheme [ADC(2)x], which involves only the lowest two excitation classes (i.e., one-hole [1h] and two-hole-one-particle [2h1p]) with respect to neutral ground state in the wave function expansion. At this level, the 2h1p-like states (shake-up ionization satellites or dicationic decay channels states with an electron in continuum) are seriously undercorrelated compared to the 1h-like main ionic states, which can affect accuracy of the calculated decay widths. Furthermore, decay processes in which 3h1p-like shake-up dicationic channels play an important role (e.g., Auger decay of the Kr 3d vacancy) or multi-electron effects such as double Auger decay cannot be studied at all using the ADC(2)x scheme.

To remedy these issues, we have developed ADC(2,2) scheme [5] in which the shake-up states are treated consistently with the main ionic states through the second order of perturbabion theory. Comprising also the 3h2p excitation class, the resulting Fano-ADC(2,2) method provides access to the second-order decay processes with two electrons in the continuum. Furthermore, the ADC(2,2) scheme itself offers unprecedented consistency in the description of main and satellite ionization states, and is thus valuable for the study of the inner valence regions of molecules where the 1h and 2h1p characters of states are usually strongly mixed due to the so-called molecular orbital picture breakdown. We will present the Fano-ADC(2,2) method and demonstrate its performance on several examples of multi-electron decay processes for which the common ADC(2)x scheme is inadequate.

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Imaging Ultrafast Chemical Dynamics

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Studying molecules and clusters in the gas phase allows for the observation and understanding of fundamental physical processes, which could be later used as a guide in order to explain more complex phenomena. To that end, we will present our results using several experimental techniques, like velocity map imaging (VMI) [1,2], x-ray coherent diffractive imaging (XCDI) [3], as well as laser-induced electron diffraction (LIED) [4]. In addition, sophisticated pump-probe experiments allow to follow the induced dynamics of such systems in real time [5]. Further results on strongly oriented or aligned molecules in field-free space [6], using shaped pulses, will also be discussed. In order to achieve high sample purity, strong inhomogeneous electric fields are applied for the spatial separation of the different species present in the molecular beam [7]. The Timepix3 camera is expected to play a crucial role in the performed experiments, as one can obtain a complete picture of the dynamics by recording all the electrons and the different ionic fragments. Our results on the dynamics of N_2, from experimental work conducted at FLASH will also be presented [8].

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Probing Structural Dynamics of Molecules and Clusters Using Intense X-ray Pulses: The Case of Indole-water

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The development of x-ray free-electron-laser (XFEL) and third generation synchrotron radiation (SR) facilities, allowed for the study of molecular dynamics within the (sub)picosecond timescale. In the present work, preliminary results on the photo-physics of indole-water$_1$ clusters [1], using a UV-pump x-ray-probe scheme, at the Linac Coherent Light Source (LCLS), will be presented. Indole (C_8H_7N) [1] is the chromophore of the amino acid tryptophane and a key component in the UV radiation damage and protection of proteins, as is the strongest near UV absorber. Upon x-ray ionization of the cluster, the different ionic fragments were collected using a Velocity Map Imaging (VMI) spectrometer. The yield of each observed fragment has been studied as a function of the delay between the pump and the probe pulses. The transfer of a H atom from the indole moiety to water was observed through the detection of H_3O^+ fragments, as was the case for the indole-ammonia cluster [3]. A detailed picture of the dynamics taking place will be presented on the poster.

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Production of an Erbium Dipolar BEC in a Tuneable Lens Optical Dipole Trap

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We describe the production of a Bose-Einstein condensate (BEC) of erbium atoms in a variable geometry optical dipole trap (ODT), employing a pair of focus-tuneable lenses, as a step towards creating a degenerate dipolar quantum gas in an optical box potential.

Our initial cooling protocol follows standard methods - a narrow line magneto-optical trap (MOT) is loaded using a Zeeman-slowed atomic beam. For transfer of atoms to the ODT we exploit the tuneable geometry to optimise the overlap between the ODT and the MOT, while retaining the ability to compress the ODT for efficient evaporation. We currently transfer $\sim 10\%$ of the $\sim 10^8$ atoms in our MOT into the ODT and then reach the BEC transition in a crossed beam ODT with $\sim 10^5$ Er atoms remaining. The tuneable lenses allow us to translate the ODT focus and so transport the atoms 40 cm to an all-glass cell for loading into a pancake optical box trap. In parallel, the experiment is being expanded to add potassium as a second atomic species. We discuss the outlook for new studies that this experiment opens up.

S2-P30

Stationary, dynamic and thermal properties of flattened and elongated quantum droplets

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We present our findings with regards to the theoretical description of quantum droplets that differ from the usual bulk form by being flattened, elongated, or at nonzero temperature. We show problems which arise while trying to describe thermal effects in quantum droplets (and Bose gases in general) and our proposition on how to deal with them. We compare the droplet stability at zero and finite temperatures. We demonstrate an effective low dimensional theory for description of the quantum droplets in the flattened and elongated regimes. As a benchmark of the effective theory, we studied droplet dynamics in the case of collisions, showcasing similarities and differences compared to regular 3D droplet collisions.

Studies in View of Positronium Laser Cooling

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AEgIS goal is to test the Weak Equivalence Principle for antimatter by measuring the free fall of neutral antihydrogen. Antihydrogen is produced [1] by using the charge exchange reaction between cold antiprotons provided by the Antiproton Decelerator (AD) at CERN and positronium laser-excited to Rydberg-levels. One of the crucial factors limiting the antihydrogen production is the velocity of positronium atoms. By cooling them, one can boost the antihydrogen production tremendously. Cold positronium also would allow one to improve positronium spectroscopy and beam formation experiments with high precision.

Positronium is produced by implantating positrons into a nanochanneled porous silicon converter [2]. Detection of positronium is done by single-shot positron annihilation lifetime spectroscopy (SSPALS). By integrating the delayed part of the signal, it is possible to extract the amounts of surviving and annihilated fraction of 1^3S positronium before and after laser manipulations.

For positronium laser cooling, the transition $1^3S \longrightarrow 2^3P$ is used as the lifetime for the 2^3P is 3.1 ns, which allows for many cooling cycles in the 142 ns lifetime of 1^3S positronium [3]. In order to probe the velocity distribution before and after the manipulation, a second independent laser is used to excite positronium from 1^3S to 3^3P, from where it is subsequently ionized by a 1064 nm laser pulse synchronized to the nanosecond. Scanning the wavelength of this laser allows one to remove parts of the positronium population with different velocities due to the Doppler shifts and therefore enabling us to reconstruct the Ps velocity distributions [4].

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Control of Electromagnetically Induced Transparency Patterns in Rydberg Media by Orbital Angular Momentum Fields

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Coherent control of atom-light interactions is an active research area in quantum and nonlinear optics. A good example of such a control is electromagnetically induced transparency (EIT) - a quantum interference effect leading to strong modification of the optical properties of the medium [1]. EIT has been studied in various multilevel atomic systems with various configurations, and recently attracted a strong interest for the applications to Rydberg atomic systems. The highly excited Rydberg atoms exhibit extreme polarizabilities and long-range interactions that give the opportunities to explore coherent phenomena in the entirely new regime [2]. In this work a spatially dependent EIT has been studied in the ensemble of cold interacting Rydberg atoms controlled by the optical vortex fields. The spatial patterning has been realized by considering Rydberg atoms in a typical three level ladder scheme and using a special control field combinations as a superposition of two Laguerre-Gaussian modes. In this setup, where different vortex control field modes are superimposed, the resulting field develops various spatially coherent structures depending on the corresponding orbital angular momentum (OAM) values of the interfering control fields. As a result, the optical response exhibits the formation of different types of bright and dark Ferris wheel structures as can be seen in the absorption patterns (Fig. 1). This setup effectively converts phase information of the optical field into intensity profiles and related modified optical response that, within the specific range of parameters, may be used to produce highly localized distributions [3]. The findings show possibility of precise spatial patterning of Rydberg atoms in the transverse two-dimensional space enabling the formation of strongly localized optical lattices with the tunable barriers between sites and providing single-site addressability for the arrays of trapped atoms.

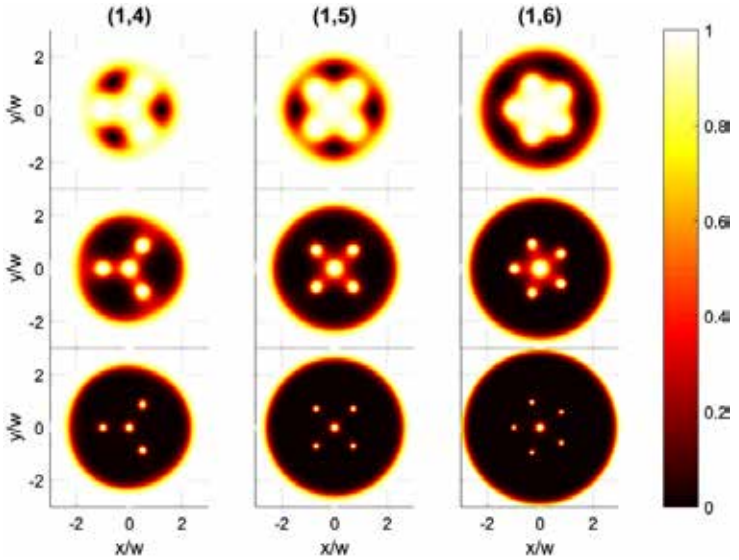

FIG. 1: Normalized transverse absorption patterns in Rydberg atomic ensemble arising from different control field OAM number combinations and for different control field amplitudes.

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Single-shot measurements of phonon number states using the Autler-Townes effect and composite pulses

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Quantum technologies employing trapped ion qubits are currently some of the most advanced systems with regards to experimental methods in quantum computation, simulation and metrology. This is primarily due to the excellent control available over the ions' motional and electronic states. By treating the ions as composite quantum systems, with qubit states that can be addressed by optical laser or microwave pulses and motional states that can be manipulated by driving sideband transitions, it is possible to engineer unique multi-qubit gate schemes for computation, simulate atom-cavity dynamics and study the boundary between classical and quantum behaviour.

In this work, we present a method for detecting the motional Fock state of a single $^{88}Sr^{+}$ ion confined in a linear Paul trap using Autler-Townes effect. In the experiment, the ion is illuminated with a light field that couples it to a phonon-number changing transition while another light field is applied to probe the Autler-Townes splitting whose magnitude is dependent on the motional state of the ion. We demonstrate this dependence for coupling to both red- and blue-sideband transitions and it is in good agreement with the theoretical model. In principle the method can be applied to any system where a quantum harmonic oscillator can be coupled to a three level system.

In addition, we introduce another method for Fock state detection relying on composite pulse sequences. We compare it with the one using Autler-Townes effect in terms of effectiveness and efficiency in being able to discern between adjacent Fock states with high accuracy. During both detection sequences the state of the system is only disturbed when the correct Fock state is revealed. Thus it is not necessary to perform individual measurements on each phonon-number state; rather a single detection sequence efficiently checks each Fock state from n=0 to n=8 non-destructively until the actual phonon number is reached.

S2-P34

Experimental investigation of the core-level ICD efficiency as a function of the number of neighbors

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Non-local decay mechanisms play an important role in the relaxation of dense media such as biological samples. Rare gas clusters can be used as a prototype system for experiments to explore these mechanisms in a less complex environment. One such non-local relaxation pathway is the Interatomic Coulombic Decay (ICD), an electronic decay mechanism which was theoretically predicted in 1997 and experimentally confirmed in 2004 [1,2]. Ever since, this field of research is rapidly growing. To estimate the impact of these non-local processes on complex samples, it is important to know the efficiency compared to local relaxation pathways. Theoretical studies show a growing ICD efficiency with the number of nearest neighbors, but there has been no experimental proof so far [3].
Here, we use the decay of a 3*d* vacancy in Kr clusters to compare the well-known MNN-Auger decay [4] to the competing core-level ICD, which has just recently been observed for the first time in van der Waals clusters [5]. In the dominant relaxation pathway, the 3*d* photoionization is followed by an Auger decay leaving the ion in a one-site dicationic ground state $4p^{-2}$. In the competing core-level ICD energy is transferred to the neighboring atom leading to a two-site dicationic state $4p^{-1}4p^{-1}$ followed by Coulomb explosion of the cluster.

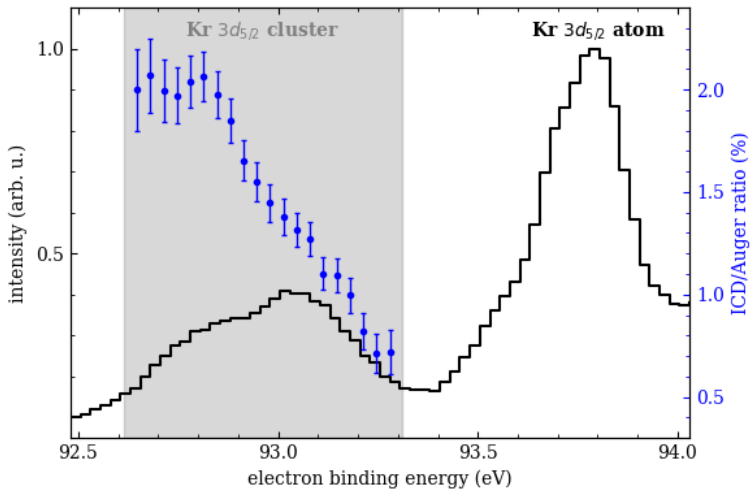

Figure 1 *Spectrum of the Kr $3d_{5/2}$ photoelectron measured in coincidence with Auger or core-level ICD electrons for atoms and clusters in a partially condensed cluster jet. The blue dots depict counts of the ICD electron signal divided by the counts of the competing Auger electron signal as a function of the photoelectron binding energy in percent.*

In a large cluster atoms at different sites have a different number of neighbors depending on the position in the icosahedral structure – from 6 for corner atoms to 12 for bulk atoms. Differences in the screening due to its dependency on the number of neighboring atoms results in a site-specific variation of electron binding energy in a cluster. This allows for a site-specific survey using the photoelectron spectrum, from which one can indirectly deduce the number of neighbors of the electron-emitting atom in the cluster.
We determined the ratio of ICD to Auger electrons in coincidence with the photoelectron by varying 0.1 eV steps across the cluster signal going from bulk to corner atoms. The resulting ratio in dependence on the cluster site and therefore the number of neighbors is shown as blue dots in Fig. 1. We observe a significant decrease in core-level ICD efficiency with decreasing number of neighbors from $(2.07 \pm 0.20)\%$ to $(0.75 \pm 0.12)\%$.

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Electron Dynamics and Correlations During High-Order Harmonic Generation in Be

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Strong laser pulses interacting with matter give rise to many fascinating phenomena [**1**]. One of them is the high-order harmonic generation (HHG [**2**]). Basic features of the HHG process can be described with the help of a three-step-model, which incorporates a single active electron (SAE) to be ionized, driven by the field and finally recombined with the parent ion. However, many-electron dynamics are known to be relevant in the description of strong-field phenomena. Here, we present theoretical results on HHG in beryllium atom irradiated by a 74 fs and 1850 nm linearly polarized trapezoidal laser pulse in the intermediate strong-field ionization regime with a Keldysh parameter of 0.85. In order to solve the four-electron time-dependent Schrödinger equation, we extend the time-dependent restricted-active-space configuration-interaction (TD-RASCI [**3**]) method, adapted in our previous work [**4**] to calculate the HHG spectra of He. We separate individual effects of different physical processes induced by the pulse by systematically increasing the space of active configurations.

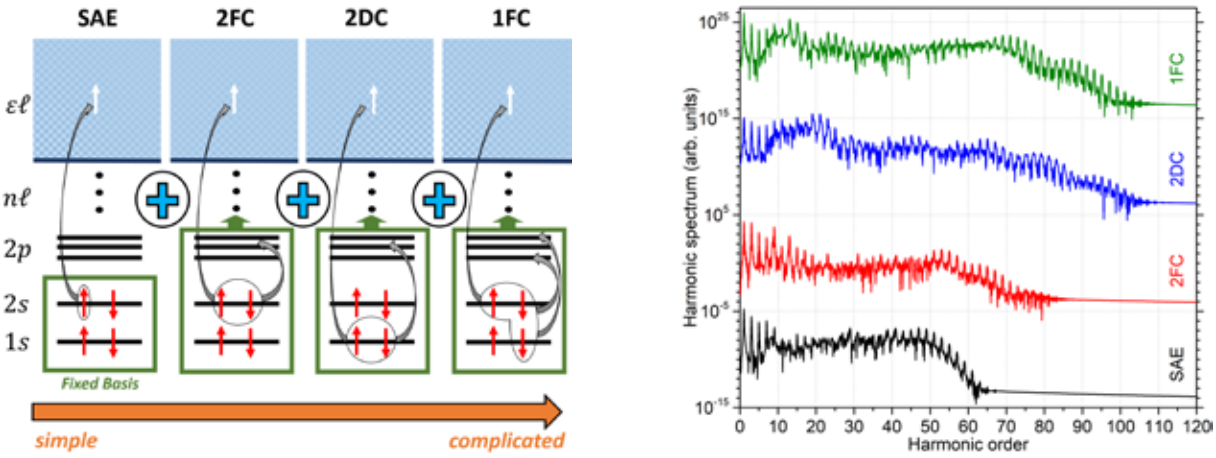

Figure 1: *Left*: Schematic explanation of approximations (with increasing complexity), which are used in this study of HHG in Be. *Right*: Computed harmonic spectra [**5**]. For a better comparison, the spectra are subsequently multiplied by a factor of 10^{10} (note the logarithmic scale of the y axis).

A schematic illustration of the used approximations is depicted on the left-hand-side, and the presently computed spectra are shown on the right-hand-side of Fig. 1. The SAE spectrum exhibits a sharp cutoff located at a harmonic order of about 60. Next, configurations with two frozen $1s^2$ electrons and two dynamically described electrons (2FC) are allowed. The respective spectrum shows already more harmonics as compared to the SAE spectrum. Going beyond the 2FC approximation is achieved by including dynamics of the $1s^2$ subshell (2DC). One can see, that photoionization of $1s^2$ enhances the computed spectrum at all harmonic orders. Finally, simultaneous dynamics of three electrons with only one electron being frozen in the $1s$ orbital (1FC) are allowed. Comparing the resulting 1FC spectrum to the 2DC one, we observe an attenuation at lower and amplification at higher harmonic orders. Thus, we obtain a significant enrichment and extension of the harmonic spectrum at all approximations beyond SAE. Strikingly, the HHG spectrum, computed at the highest level of approximation, shows harmonics up to an order of about 100. This confirms the significance of dynamics and correlations in the HHG process.

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Effect of Saturation on Hyperfine Structure Spectra in Laser Absorption Spectroscopy

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By the use of laser spectroscopy i.e. optogalvanic spectroscopy or the LIF method, it is often possible to separate and register individual components of the hyperfine structure. An analysis of the hyperfine pattern provide valuable information about the nuclear as well as the electronic structure of atoms.

Unfortunately in many cases of rich spectra the hyperfine spectrum is blended, rather than completely resolved. In these cases it is necessary to use a fitting procedure to establish the positions of the individual components. Standard techniques developed for this fitting procedure incorporate the theoretically predicted relative intensities of the individual components. However, because of the saturation effect the intensities of the individual components deviate from intensities predicted by theory and theoretically predicted shape of the spectrum does not fit the experimental results. Sometimes, it is possible to reduce the laser power to a level in which the observed intensities are in agreement with predictions, but in many cases the saturation effect cannot be avoided. Due to the saturation effect stronger components (with larger transition probabilities) have relatively lower intensities in comparison with weaker components.

The saturation effect changes the shape of the registered spectra both in the measurements of the Zeman structure and the hyperfine structure, and its influence on the recorded Zeeman structure is greater. In our most recent works (see i.e.[1]), in which we examined the Zeeman structure we have modified our computer program for the fitting procedure be able to analyze such cases. We have introduced an additional free parameter A_s (saturation rate) the value of which is determined by the fitting process. The calculated decay rate of each Zeeman component (A_ν) of frequency ν was modified in accordance with:

$$A_\nu^{sat} = \frac{A_\nu}{1 + A_\nu / A_s}. \tag{1}$$

Here A_ν is the unsaturated decay rate (resulting from the theory) directly proportional to the intensity of radiation. The key assumption behind the validity of formula (1) is the theory presented in monograph [2].

In the case of saturated hf spectra (when magnetic field B=0) the computer program calculates intensities of each individual hfs component as a sum of contributions from all M, M' components.

When measuring the hyperfine structure it is assumed that the polarization state of the exciting light has no effect on the shape of the registered structure. However this is true as long as the saturation effect is absent. In the presence of saturation effect the shapes of the spectra for the polarization π and σ are different. This is illustrated in the figure below.

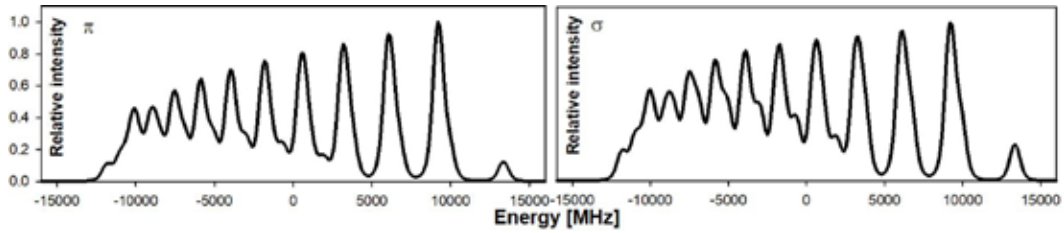

FIG. 1:An exemplary simulation of a hyperfine structure for π and σ polarization with $A_s = 10$.

Conclusion: The hyperfine structure measurements should be carried out in conditions where the polarization state of the exciting laser light is known, and this fact should be reflected in simulations that match the shape of the experimental spectrum to the theory.

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Multiple photoionization for the $2p$ shell in the iron atom

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Study of the interstellar medium (ISM) is critical in understanding the structure of the galaxy and formation of stars. High resolution X-ray spectroscopy provides an important information about abundance of the constituent elements in the ISM. The multiphase structure characterized by gas, dust and molecules can be determined through analysis of absorption lines and edges in the X-ray spectra. What is more, the lines of iron provide an important contribution to the spectra from active galactic nuclei. Theoretical multiple-photoionization cross sections were previously investigated for the K shell of the Fe atom [1] and Fe^{2+} ion [2]. However, modeling of ionization balance in photoionized plasma requires photoionization cross sections for all ions and their shells.

In continuation of our earlier work on multiple photoionization of the Fe atom and ions [1,2], here we study the multiple photoionization produced by a creation of the $2p$ shell vacancy in the Fe atom. The electric dipole transitions are investigated in the radiative decay process. Multiple-photoionization cross sections are analyzed for all 34 levels of the ground configuration of the Fe atom. The single photoionization from the $2p$ subshell is followed by radiative and Auger cascade which mainly leads to higher ionization stages. The radiative and Auger cascade is analyzed for 73 configurations (Fe^{+}: 5, Fe^{2+}: 13, Fe^{3+}: 18, Fe^{4+}: 20, Fe^{5+}: 17 configurations). These configurations correspond to 21151 energy levels: Fe^{+}: 522, Fe^{2+}: 2012 , Fe^{3+}: 5577, Fe^{4+}: 7619, Fe^{5+}: 5421.

The multiple-photoionization cross sections for the ground level of the Fe atom are presented in Fig. 1. The states of the Fe^{+} - Fe^{5+} ions are produced in the photoionization process. The quadruple-photoionization cross sections are above the ones of the triple photoionization approximately by a factor of two. The single-photoionization cross sections are by two orders of magnitude lower compared to the quadruple-photoionization cross sections.

The similar situation is obtained for the multiple-photoionization cross sections from the highest level of the ground configuration of the Fe atom (not presented here). The quadruple-photoionization cross sections also prevail for this level. On the other hand, the cross sections to Fe^{4+} are $\sim 10\%$ higher for the ground level compared to the highest level of the ground configuration. What is more, difference among peak values of the quadruple-photoionization cross sections from the different levels of the ground configuration is $\sim 14\%$. The partial photoionization cross sections from the ground level of the Fe atom to configurations of the produced ions are also analyzed in the study.

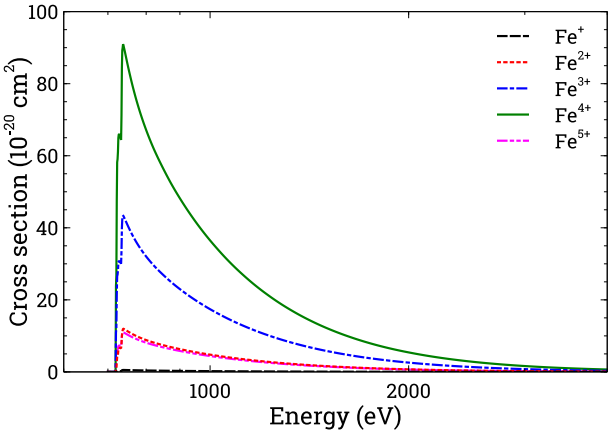

FIG. 1: Multiple-photoionization cross sections for the ground level of the Fe atom.

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Spectroscopy of Potassium Complexes in Helium Droplets: From Molecular Transitions to Plasmon Modes in Nanoparticles

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We explore the evolution of the electronic spectrum of potassium clusters isolated in helium droplets from single atoms and molecules up to nanometer sized particles. [1] A supercontinuum laser equipped with a tunable filter is used to excite the potassium clusters, the employed method is sketched below. The excitation of potassium complexes results in a rapid dissipation of the energy introduced to the system by the evaporation of helium atoms. This translates into a depletion of the helium flux that can be detected by a mass spectrometer. Small potassium molecules exhibit multiple distinct spectral features, known dimer and trimer transitions can be readily assigned. Beyond a cluster size K_n of about $n = 20$, the depletion spectra are dominated by a single, broad feature at about 600 nm, which corresponds to the collective resonance of the isolated potassium clusters. With increasing cluster size, this resonance continuously shifts towards the blue. For larger clusters K_n with a size of about $n = 600$, a splitting of the plasmon mode into two components is observed. Supported by simulations, this observation is explained by the presents of elongated nanoparticles in helium droplets that are formed in a multi-center aggregation process. The presented, supercontinuum laser-based experimental approach opens the door for the spectroscopic characterization of many different materials and material combinations isolated in helium nanodroplets [2, 3], in a size regime ranging from single atoms and molecules to small sub-10 nm particles.

The achievable resolution in the beam depletion spectroscopy experiments is limited by the relatively broad linewidth of the supercontinuum laser of about 6 nm. By employing laser induced fluorescence spectroscopy we show that vibrationally resolved spectra can be recorded for potassium dimers and trimers, which desorb from the surface of the helium droplet upon excitation.

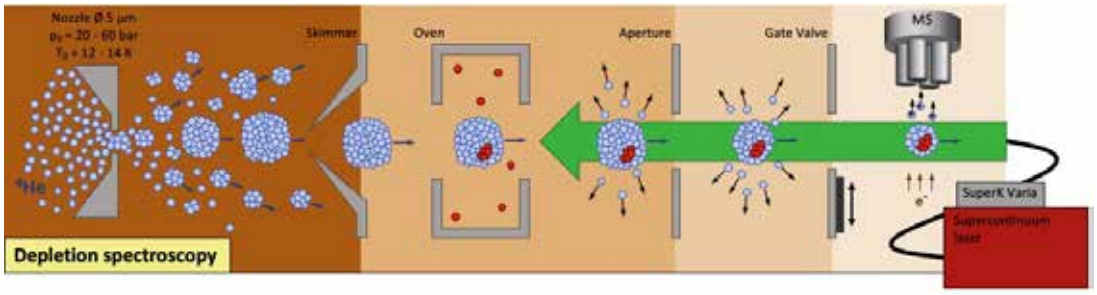

FIG. 1: Sketch of the beam depletion spectroscopy approach employed for the investigation of potassium complexes isolated in helium droplets.

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Anisotropy of Multiple-Quantum Fluorescence Signals in Dilute Atomic Vapors

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We investigate collective effects in thermal atomic alkali vapors by multiple-quantum coherence (MQC) experiments, where multiphoton processes can be separated from one-photon transitions and can be assigned to specific particle numbers [**1**, **2**]. The technique is sensitive enough to reveal weak interparticle interactions, despite the thermal motion and the spatial separation of the atoms in the micrometer-range [**3**]. We experimentally investigate the dependence of such signals on the laser polarization and compare the results to calculations using a theoretical model, which describes MQC signals by scattering processes of real photons [**4**, **5**].

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Full quantum control over randomly oriented chiral molecules

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Enantiomer separation, conversion and purification of chiral molecules in the gas phase by means of electromagnetic fields is an open challenge. The random orientation of molecules in the gas phase, which is reflected in the degeneracy of the rotational states, implies a symmetry that must be completely broken by the external fields. We show how to apply controllability analysis to quantum asymmetric tops [1,2] in order to determine the number, polarization and frequencies of the external fields which are required to fully control the rotational or ro-vibrational dynamics of randomly oriented chiral molecules. The results of the controllability analysis allow us to design pulse sequences which drive the molecules to the desired target states.

We demonstrate this strategy for two examples. Enantiomers of rigid chiral molecules can be excited selectively by microwave three-wave mixing [3,4]. We present a modified three-wave mixing scheme that allows for complete enantio-selective population transfer despite the degeneracy of the rotational states [1] and thus increases the efficency of microwave three-wave mixing experiments. Chiral properties can also be observed in achiral molecules. To demonstrate this, we show how to create a chiral vibrational wavepacket in randomly oriented planar molecules.

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Electron affinity and lifetime measurements of negative ions

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Negative ions are unique quantum systems to probe electron correlation effects: since the Coulomb potential of the nucleus is almost entirely screened, the binding of the additional electron is primarily due to many body interactions between electrons. Consequently, negative ions are sensitive probes for electron correlation theories that go beyond the independent particle approximation, which is of crucial importance for the understanding of atomic and molecular structure. However, due to the weak binding potential, the energy gained by attaching an electron to a neutral atom, referred to as electron affinity (EA) is typically only in the order of one eV. For the same reason, negative ions typically lack bound excited states with opposite parity, noticeable exceptions being lanthanum, cerium, osmium and thorium [1-4]. Consequently, the EA is the only parameter which can be probed with high precision, typically via laser photodetachment threshold spectroscopy.

In order to fully characterise the structure of a negative ion, individual detachment channels can be investigated using a resonance laser ionisation scheme for detection[5], whereas measurements of angular distributions of the outgoing electron can give insight into the electronic states [6], including recent developments utilising velocity map imaging to recreate the three dimensional distribution of photoelectrons [7]. Furthermore, lifetime studies of metastable and doubly excited states of negative ions can be performed in storage rings such as the Double ElectroStatic Ion Ring ExpEriment (DESIREE) in Stockholm, Sweden [8].

Here, we will present the results of lifetime and EA measurements of arsenic and rubidium as well as giving an outlook on future activities, including the commissioning of a velocity map imaging spectrometer.

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Compressibility and the equation of state of an optical quantum gas in a box

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The compressibility of a medium, quantifying its response to mechanical perturbations, is a fundamental quantity determined by the equation of state. For gases of material particles, studies of the mechanical response are well established, in fields from classical thermodynamics to cold atomic quantum gases. In the quantum degenerate ideal Bose gas in two dimensions, however, a peculiar prediction so far has remained unseen: the compressibility of the gas is expected to become infinitely large. Here we demonstrate a measurement of the equation of state as well as the compressibility of a homogeneously trapped two-dimensional quantum gas of light inside a nanostructured dye-filled optical microcavity. Upon reaching quantum degeneracy we observe signatures of Bose-Einstein condensation in the finite-size system, causing a sharp increase of the density response to an external force, hinting at the infinite compressibility of the uniform two-dimensional Bose gas.

Entanglement of the macroscopic spins of two spatially separated Bose-Einstein condensates

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We experimentally investigate the entanglement of two spatially separated many particle systems. Our experiments are based on a two component pseudo spin-1/2 Bose Einstein condensate of ^{87}Rb on an atom chip. By engineering the interatomic interactions through state dependent trapping we are able to produce entangled spin-squeezed states in this system. Using coherent spin manipulation we split this entangled many-particle state into two halves in spin space and magnetic field gradients allow us to separate the two two-component BECs spatially by more than 40 μm. Our technique allows us to individually address the collective spins of the two BECs after splitting thereby realizing arbitrary spin measurements on the two systems. Their correlations allow to infer measurement results of non-commuting spin observables in one system from measurements on the other, demonstrating the entanglement of the two Bose-Einstein condensed clouds of roughly 800 atoms each. Besides the interest in understanding fundamental aspects of entanglement of many-body systems our experiments enable new investigations in quantum enhanced metrology using spatially split probes.

Synthetic Gauge Potentials for the Dark State Polaritons in Atomic Media

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The quest of utilizing neutral particles to simulate the behavior of charged particles in a magnetic field makes the generation of the artificial magnetic field of great interest. We put forward an optical scheme to generate effective gauge potentials for stationary-light polaritons in the static laboratory frame. To demonstrate the capabilities of our approach, we present a recipe for having dark-state polaritons in degenerate Landau levels. Our scheme paves a novel way towards a versatile quantum simulator for mimicking different Hamiltonians by electromagnetically induced transparency [**1**].

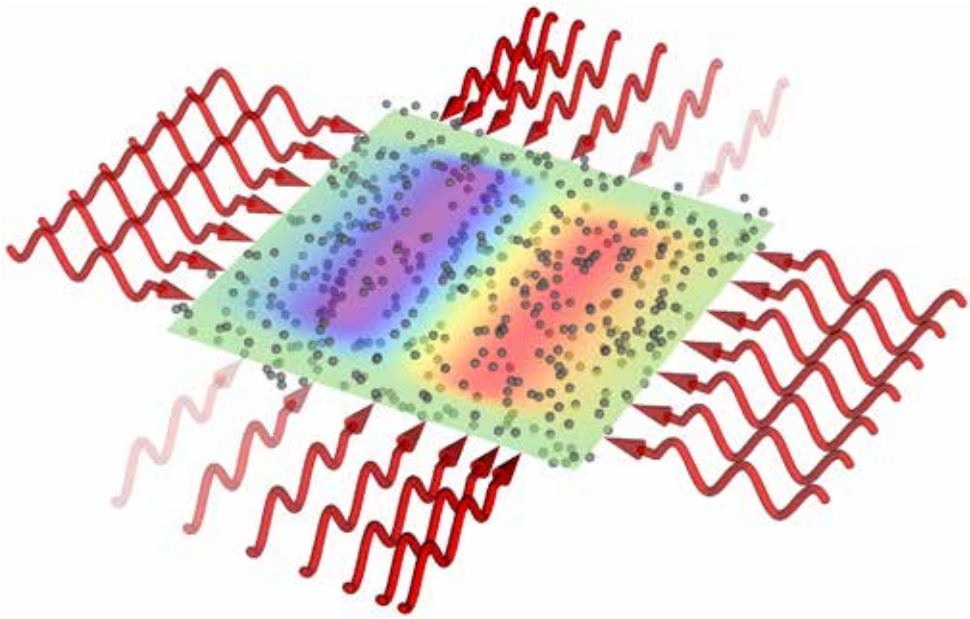

FIG. 1: Illustration for a two-dimensional electromagnetically-induced-transparency system.

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Error mitigation for quantum simulations on trap ion quantum computer

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Quantum error mitigation is a common name for all techniques aimed at reducing the effects of noise, occurring during computation, on the measurement statistics. Zero noise extrapolation is an error mitigation technique that utilizes the ability to perform computation with varying noise strengths, larger than the initial, and then using data obtained for extrapolating to the noiseless value.

We are at the early stages of many body quantum simulations on trapped ion quantum computer design using zero noise extrapolations scheme to mitigate the noise. The simulations of the time evolution of one qubit Hamiltonian presented in 1 are performed.

$$\mathcal{H} = J\sigma^z + h\sigma^x \tag{1}$$

where J is z-direction coupling and h is transverse field coupling. The time evolution is performed using the time evolution operator $u(t)$ obtained from second order Suzuki Trotter formalism and given in 2.

$$u(dt) = \exp(\frac{-idt}{2}\sigma^z)\exp(-idt\sigma^x)\exp(\frac{-idt}{2}\sigma^z) + \mathcal{O}(dt^3) \tag{2}$$

where N is number of Trotter steps and $dt = T/N$ with T final time.

To perform ZNE the circuit has to be performed at varying noise strengths. The different error strengths were obtained using two noise scaling schemes. The first scheme was unitary folding, insertion of unitary gate units inverse equal to the identity, such that the increase in a number of gates would result in increased noise level but leave the result of the computation unchanged. The second method of noise scaling used was scaling using Trotter decomposition: varying number of steps to get same time interval. For this method different numbers of steps, N were used to reach the same time point T. With an increased number of steps the number of gates linearly increases, therefore the physical error is expected to increase, while the Trotter, or algorithmic error, decreases with the decreasing time step, dt.

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XPS Study of Cu(II) complexes in solution

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The electronic structure of Transition-metal (TM) complexes has received considerable attention in both theoretical and experimental chemistry since the 50's and discovery of ferrocene. This is mainly due to the many applications of such molecules and their derivative compounds in areas such as synthesis, homogeneous catalysis,. [1]. At the center of all these processes are the ultrafast charge-transfer leading to the formation and breaking of chemical bonds. The chemical properties of TM complexes strongly depend on the type and extent of these bonding, and hence on electronic structure. With the advent of liquid-microjet method, combined with state-of-the-art synchrotron-based X-ray spectroscopy available at the PLEIADES beamline [2] of the French national Synchrotron facility, it is now possible to explore the electronic structure in aqueous environments.

we have performed photoemission experiments on 2 copper compounds ($Cu(NH_3)_4SO_4,H_2O$ and $Cu(H_2NCH_2CH_2NH_2)_2(OH)_2$). In both cases, copper has +II oxidation state in, octahedral/square plane geometries The Cu 3d as well as N 1s and the subsequent Auger decay spectra will be presented and compared.

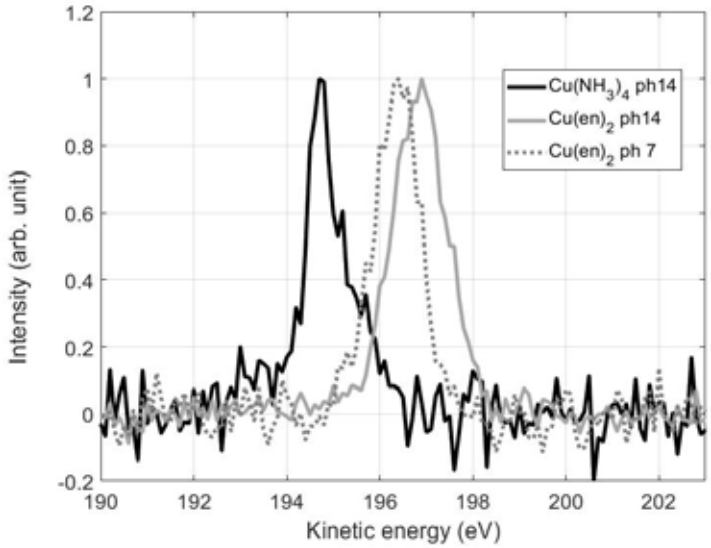

FIG. 1: XPS N 1s spectra of both Cu complexes.

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Post Collision Interaction effect studied of solvated ions ionized in K shell

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Following inner-shell photoionization of an atom or a molecule, a photoelectron is emitted ($h\nu + M \longrightarrow M^{+*} + e_{ph}$) and the short lifetime unstable state M^{+}* can relax by emission of a subsequent Auger electron ($M^{+*} + e_{ph} \rightarrow M^{2+} + e_A$). When the photon energy is just above the inner-shell ionization threshold, we have strong coulombic interaction between the Auger electron, the photoelectron, and the ionic core. Indeed, the photoelectron (which has a small kinetic energy) will feel a quick change of the ionic charge when the Auger electron (which has a high kinetic energy) overtakes it. This effect is known as *post collision interaction* effect (PCI) and leads to shifts and distortions of the photoelectron and Auger peaks in the vicinity of the inner-shell ionization threshold.

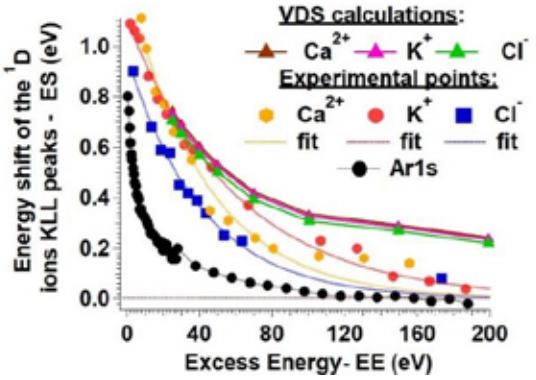

Figure 1 : *PCI shift the ^{1}D KLL peaks for the ions Cl^-, K^+ et Ca^{2+} in water in comparison with the results obtained for Ar 1s^2 and with the theory, in the vicinity of the ionization threshold of each ion studied.*

In gas phase and in the tender's X-ray domain (~1– 5 keV), this effect was observed on Argon **[1]**. A maximum shift of 0.8 eV of the main KLL Auger peak, is observed just above the 1s ionization threshold and decreases with increasing photon energy. It has been shown, in the bulk **[2],** that this energy shift could also be influenced by the modification of the effective charge of the residual ion (screening). Therefore, applied to the aqueous phase, we chose to study, by Auger spectroscopy, the PCI effect on different ions isoelectronic to Argon: Cl^-, K^+ and Ca^{2+}. For these isoelectronic ions, the $1s^{-1}$ core-hole states decay by emitting KLL Auger electrons leading to the final states of the $2p^{-2}$ configuration with ^{1}S, ^{1}D and ^{3}P terms. The experiments were conducted on the GALAXIES **[3]** beam line of the Synchrotron SOLEIL (France) on a liquid micro-jet adapted for the HAXPES **[4]** photoemission end-station. KCl and $CaCl_2$ solutions were prepared at 0.5 M. To evaluate the PCI shift, we focused on the position of the maximum of the most intense well isolated $2p^{-2}(^1D)$ peak with photon energy. For each ion, we compared the values obtained with Argon. Experimental results are presented in **figure 1 and compared to the Van Der Straten [5] calculations type (for each ion)**. The x-axis corresponds to the photon energy minus the ionization potential (nominal photoelectron kinetic energy) and the y-axis correspond to the PCI shift determined by the shift of the Auger ^{1}D peak recorded close the threshold relative to the position of this same peak recorded far from the threshold (where the photoelectron has a high kinetic energy). (ES = $E_k(^1D)$-$E_k(^1D)$ (unshifted)) and (EE= $h\nu$- I.P). The curves linked to these ions show: 1- a decrease of the PCI effect slower than in Argon, that is due to screening effect and to the reduced mean free path of the photoelectron in the liquid medium, 2- a shift slightly greater at threshold (1 eV versus 0.8 eV) and 3- a charge/size effect not very significant.

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Simulation of squeezing models with atomic fermions in optical lattices via spin-wave theory

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Significant theoretical and experimental progress in studying and understanding complex many-body physics has been made in optical lattice settings, which provide clean and controllable setups. Ultracold atomic Fermi gases in an optical lattice are used in the most precise and accurate optical lattice clocks (reaching precision record $3 \cdot 10^{-19}$ [1]), as the Pauli exclusion principle suppresses unwanted collisional frequency shifts. Furthermore, ultracold atomic gases in optical lattices are nearly perfect for realization of many condensed matter phenomena i.e., they offer various kind of Hubbard models with great flexibility of parameters [2] (Fig. 1). Recently it was suggested that the interaction among identical atomic fermions needed for the spin squeezing can be induced via the spin-orbit coupling (SOC), which is generated by means of an additional laser that drives the clock transition [3].

In this work, we investigate spin-squeezed states in an optical lattice composed of ultra-cold fermions employing position-dependent SOC that can be induced in realistic experimental conditions. By choosing an appropriate propagation direction of the laser beam inducing the SOC and acting on a fermionic lattice with a sequence of such laser pulses we expect to realize efficient spin-squeezing. The presented method might serve as a resource for quantum-enhanced metrologically useful correlated many-body fermionic states, and it might deliver gains in real applications like optical clocks.

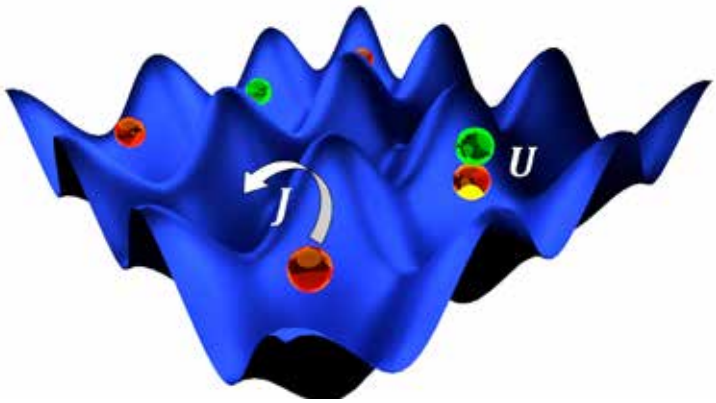

Figure 1: A Fermi-Hubbard model with ultracold atoms trapped in the lowest band of an optical lattice. Due to Pauli's principle, tunnelling between lattice sites J is only possible if the final lattice site is empty or occupied with an atom with a different spin. Two atoms with opposite spin localized at the same lattice site have an interaction energy U. The J/U ratio and the filling determines the physics of the system.

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Burst-mode filamentation and supercontinuum generation in transparent solids

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Burst trains of femtosecond pulses emerge as a powerful tool for laser material processing, offering a variety of innovations in micromachining of metals [1], polymers [2] and glasses [3]. On the other hand, burst-mode operation enables efficient power scaling of few optical cycle optical parametric amplifiers [4] and OPCPA [5], which may further serve for seeding high repetition rate free-electron lasers. The generation of few optical cycle pulses requires ultrabroad spectral bandwidths, which are readily produced by supercontinuum generation via self-focusing and filamentation of intense femtosecond pulses in transparent solid-state materials [6]. However, filamentation phenomena with femtosecond pulse bursts are still poorly studied, especially for what concerns heat and defect accumulation that modify linear and nonlinear optical properties of the material that in turn alter filamentation dynamics.

In this Contribution we report the results of high repetition rate burst-mode femtosecond filamentation and supercontinuum generation in sapphire and YAG crystals. The experiments were performed using an amplified Yb:KGW laser (Carbide, Light Conversion Ltd.), which provided bursts of 210 fs, 1030 nm pulses at 1 MHz repetition rate with intra-burst repetition rates of 69 MHz and 2.5 GHz. The time evolutions of relevant filament parameters: supercontinuum spectra, filament-induced luminescence tracks and crystal temperature were measured in various operating regimes, which were accessed by changing the number of pulses (from single pulse to 10 pulses per burst) and intra-burst repetition rate. Short-term (over 10 min.) measurements demonstrated stable supercontinuum generation in all the investigated settings, however, as compared to a single pulse case at 1 MHz, burst-mode operation revealed a considerable increase of crystal temperature up to 69 degrees in sapphire and to 33 degrees in YAG alongside evident onset of thermal lensing, as verified by monitoring of filament-induced luminescence traces.

Our results are important for building better understanding of ultrafast nonlinear light-matter interactions with femtosecond pulse bursts in general, and for practical realization of durable, modification-free burst-mode supercontinuum generation in solid-state materials, in particular.

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Quenching of Photon Emission in Interatomic Decay of Heterogeneous Noble Gas Clusters After Direct Double Photoionization and Innershell Ionization

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With the theoretical proposal and subsequent experimental verification of non-local decay mechanisms like the interatomic coulombic decay (ICD), significant progress has been made within the recent years towards an understanding of the role of an environment in possible relaxation pathways (see [1] and references therein). ICD and related phenomena like ETMD have been discussed as possible causes for radiation damage in cells as they lead to the emission of slow electrons, which – unlike faster Auger electrons – are more likely to be mutagenic. Even very weak bonds, like van-der-Waals bonds, enable these non-local decay mechanisms, making noble gas clusters well-suited prototype systems for the investigation of such fundamental atomic and molecular processes.

Here, we present our state-of-the-art experiment where both electrons and photons were detected in coincidence, which allows for investigation of multi-particle decay pathways after excitation with synchrotron radiation. The initial dicationic state to induce the decays is prepared in two ways, by direct double photoionization and by inner-shell photoionization and subsequent autoionization (Auger decay). The results show that the addition of a heavier noble gas to the homogeneous clusters strongly alters the emission by the opening of a faster ionizing decay channel compared to the radiative decay. Fig. 1 shows the quenching effect in neon-krypton clusters after direct double photoionization, where the signal vanishes when considering a photon coincidentally measured with the two photoelectrons.

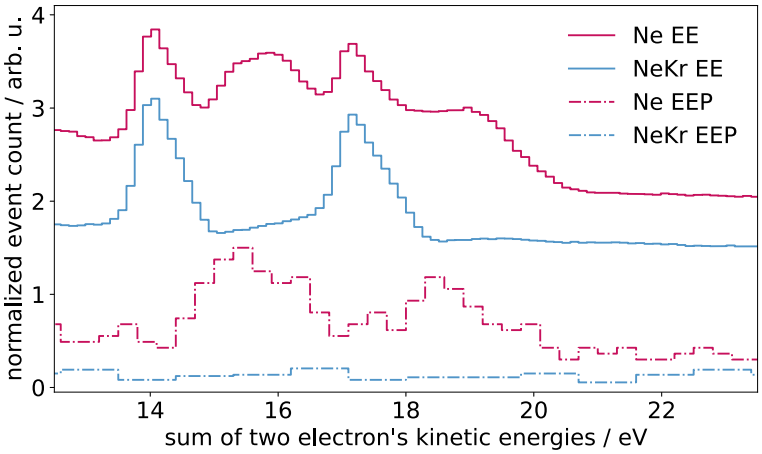

FIG. 1: Normalized number of events after direct double photoionization in pure neon and mixed neon-krypton clusters. The cluster signal at around 15.5 and 19 eV is quenched in the heterogeneous system when filtering for a photon measured in coincidence with the photoelectrons (EEP).

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Theoretical study of the ℓ-dependence of the autoionization rates of core-excited Rydberg states

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Atoms and molecules in a core-excited Rydberg state possess one electron excited to a high-lying orbital whereas the residual ion core is in a low-lying excited state. They are energetically above the first ionization threshold and can decay rapidly by autoionization. It is well known that the autoionization rates decrease with the principal quantum number n of the Rydberg electron as $1/n^3$. Their scaling with the Rydberg-electron orbital-angular-momentum quantum number ℓ, on the other hand, is unknown [1, 2]. We present a theoretical study of the autoionization rates of the core-excited Rydberg states of alkaline-earth-metal atoms for a broad range of n and ℓ values. Such species possess only two valence electrons, which makes extensive and accurate calculations feasible. The core-excited Rydberg states of alkaline-earth metals have promising applications in the fields of quantum simulation and quantum-information processing [2, 3], for which a detailed knowledge of the autoionization rates is required. A better understanding of the ℓ-dependence of the autoionization rates is also important to estimate more accurately the autoionization lifetimes of Stark-mixed Rydberg states, such as the ones used for pulsed-field-ionization zero-kinetic-energy photoelectron spectroscopy, as well as dielectronic recombination rates. We performed large-scale calculations of the autoionization rates of Mg, Ca and Sr using the method of configuration interaction with exterior complex scaling (CI-ECS) [4]. CI-ECS allows the treatment of the two-valence-electron dynamics in its full dimensionality and does not rely on the assumptions made in other widely used methods [4]. Diagonalization of the complex-scaled Hamiltonian calculated using numerical basis functions directly provides the autoionization rates of the core-excited Rydberg states, which are twice the imaginary part of the complex eigenvalues. Our first results agree with the rapid decrease of the autoionization rates with ℓ observed in other studies (see, e.g., Refs. [1, 2]) and a detailed characterization of this behavior with respect to all relevant angular-momentum quantum numbers is under way.

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Absolute cross sections and asymmetry parameters for photodetachment of excited $C^-(^2D)$

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Negative ions are of fundamental interest for the understanding of electron correlation and also play an important role in domains such as astrophysics and atmospheric physics. Until recently, the photodetachment of the ground state of the carbon anion C^- (^4S) suffered from long-standing discrepancies between the results of different calculations as well as between theory and experiment. New theoretical and experimental results were reported in [1], which are in very good mutual agreement, as well as a new description of the resonant process occurring for photon energies around 6 eV. Following on from of our previous work, we report here the results obtained for photodetachment of the excited state (^2D) of C^-, in particular over the photon energy range from 0.5 to 2.5 eV where the disagreement between existing calculations are particularly pronounced [2, 3].

A new theoretical description of the photodetachment process is provided, based on an R-matrix approach employing a basis set including polarized pseudostates to reproduce the polarizability of the carbon ^3P ground state. For the first time, absolute experimental cross sections have been obtained over the whole range, by the use of a modified Animated Crossed Beam (ACB) technique allowing for the presence of multiple components in the beam, while proper differential cross sections in the same range have been measured using our Velocity Map Imaging (VMI) spectrometer.

We have also determined a more precise value for the electron affinity (EA) of the excited state, which is slightly higher than the pioneering experimental value of [4] and thus in strong disagreement with theoretical predictions of [5] and [3].

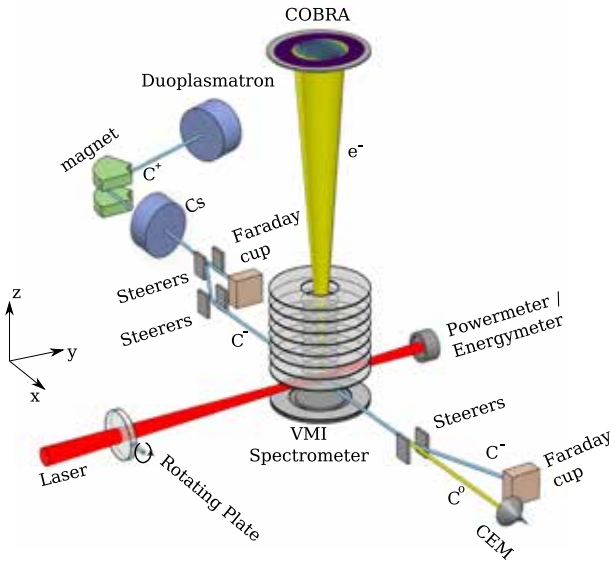

FIG. 1: Experimental setup. The ^{2}D population is generated by double electron capture of C^+ on Cs.

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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, 6.5×10^{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

$$A(D) = \frac{N(D) - N(-D)}{N(D) + N(-D)} \tag{1}$$

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

$$A(E, \varphi_{CEP}) = \frac{N^+(E, \varphi_{CEP}) - N^-(E, \varphi_{CEP})}{N^+(E, \varphi_{CEP}) + N^-(E, \varphi_{CEP})} \tag{2}$$

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 4×10^{12}W/cm^2 intensity. We found that the left-right asymmetry is more pronounced for pulses shaped with positive Group Delay Dispersion (GDD). It was also found that shaping a pulse with increasing amounts of GDD in absolute value blurs the CEP dependence, which is attributed to the increasing number of optical cycles.

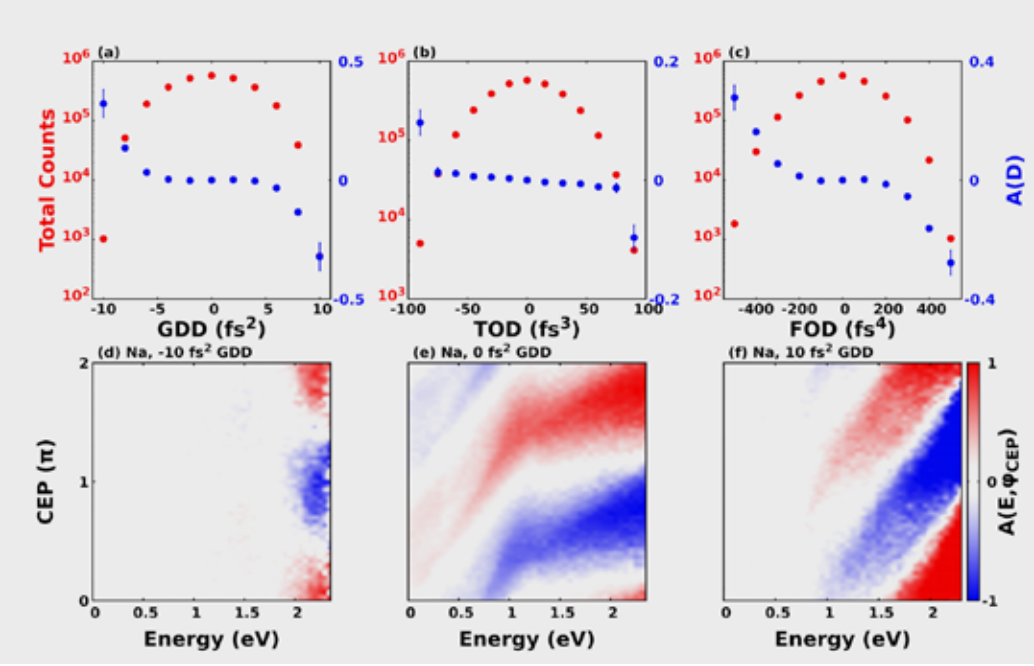

FIG. 1: Number of electron counts and asymmetry parameters for hydrogen calculated with different GDD (a), TOD (b) and FOD (c). Calculated maps of the asymmetry defined by Eq. (2) for Na at 4×10^{12}W/cm^2 intensity with different values of GDD (d)-(f).

Cyclic Einstein-Podolsky-Rosen steering

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Einstein-Podolsky-Rosen (EPR) steering is a form of quantum correlation that exhibits a fundamental asymmetry in the properties of quantum systems. Given two observers, Alice and Bob, it is known to exist bipartite entangled states which are one-way steerable in the sense that Alice can steer Bob's state, but Bob cannot steer Alice's state. Here we generalize this phenomenon to three parties and find a cyclic property of tripartite EPR steering. Specifically, we identify a three-qubit state whose reduced bipartite states are one-way steerable for arbitrary projective measurements. This tripartite quantum state exhibits cyclic EPR steering in the sense that each party can steer the state of the party to the right of it, but not the state of the party to the left to it.

The concept of steering was introduced by Schrödinger in 1935 [1], and more recently has emerged as a novel form of quantum correlation in between quantum entanglement and Bell nonlocality [2]. To elucidate the concept, consider two observers, Alice and Bob, who share the maximally entangled singlet state $|\psi^-\rangle = (|0\rangle_A |1\rangle_B - |1\rangle_A |0\rangle_B)/\sqrt{2}$. Alice by measuring her particle projects her share of the state into $|v_A\rangle = a\,|0\rangle_A + b\,|1\rangle_A$. Bob's state then immediately collapses to the orthogonal state $|v_B\rangle = -b^*\,|0\rangle_B + a^*\,|1\rangle_B$, where $*$ means complex conjugation. Therefore, Alice can prepare different states on Bob's part by suitably adjusting the coefficients a and b of her measurement. That is, Alice can steer Bob's state.

It was a natural question whether one-way EPR steering existed [2]. Namely, are there asymmetric entangled states where steering from Alice to Bob is possible, but not the other way around? This would be a weak form of steering, where the role of observables would be fundamentally different. Note that such a phenomenon cannot occur for pure entangled states, like in the above case of singlet state $|\psi^-\rangle$, because a pure state can always be brought into symmetric form by a suitable modification of the local basis. Therefore, one-way EPR steering requires the existence of mixed entangled quantum states. Indeed, it was shown that one-way EPR steering occurs for special families of two-qubit mixed states considering arbitrary projective measurements [3], and the proof was later extended to the case of general POVM measurements [4].

In this work, we generalize the phenomenon of one-way EPR steering phenomenon from two parties to three parties and find a cyclic property of EPR steering [5]. In particular, we propose a three-qubit cyclic translationally invariant ansatz state and optimize its coefficients. As a result of a heuristic search, we find a three-qubit state with the following properties: (i) All reduced two-qubit states are one-way EPR steerable for arbitrary projective measurements, where we used numerical techniques recently developed by Nguyen et al. [6] to prove steerability. (ii) The three-qubit state has a cyclic steering property in the sense that, when the system is arranged in a triangular configuration, the neighboring parties can only steer each other's states in one (e.g., clockwise) direction. That is, Alice can steer Bob's state, Bob can steer Charlie's state, and Charlie can steer Alice's state, but not the other way around. We have thus shown a peculiar directional feature of tripartite quantum correlations, which can neither appear in the phenomenon of quantum entanglement nor in standard Bell nonlocality.

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Electronic *g*-Tensor Dependence on the Size of Nanodiamonds: A Test for Geometries Obtained with GFN2-xTB Method

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Nanodiamonds (NDs) are carbon-based nanomaterials that recently gained plenty of attention in such biomedical areas as tissue engineering, labelling, and drug delivery [1]. Interestingly, a combination of drug delivery with the bioimaging capabilities could make NDs a very promising platform for the clinical theranostic applications, thereby allowing even more effective exploitation of these nanoparticles.

In order to successfully utilize the bioimaging potential of NDs, one has to be aware of their magnetic properties determined by the introduced point defects. In this work, density functional theory calculations were performed to find out the influence of the size of NDs on their electronic *g*-tensor values, with the emphasis put on the accuracy of the geometries of NDs obtained by applying computationally light GFN2-xTB method developed by Stefan Grimme's group [2].

Several point defects, including nitrogen-vacancy, silicon-vacancy, germanium-vacancy, and nickel-vacancy centers that are especially attractive for biomedical applications [3], were incorporated into fully hydrogenated and octahedrally shaped NDs of C_{84}, C_{165}, and C_{286} size (see a visualization of NDs in Fig. 1), as hydrogenation is one of the most popular surface functionalization schemes [4], while octahedron is one of the most common shapes of NDs [5]. Analysis of the obtained results not only reveals how electronic *g*-tensor values change with the size of NDs but also whether geometry optimization employing very fast GFN2-xTB method could be recommended for the investigation of much larger systems.

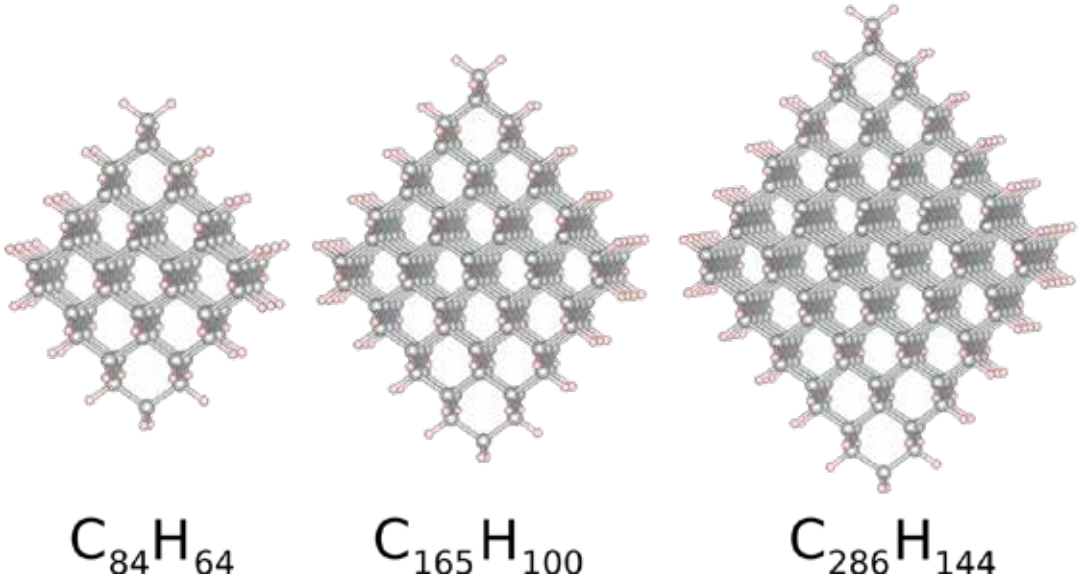

FIG. 1: Hydrogenated and octahedrally shaped NDs of different size.

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Control Of Kerr Nonlinearity In A Four-Level Quantum System Near A Plasmonic Nanostructure

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We investigate the nonlinear optical response of a four-level double-V-type quantum system interacting with a pair of weak probe fields while located near a two-dimensional array of metal-coated dielectric nanospheres. Such a quantum system contains a V-type subsystem interacting with surface plasmons, and another V-type subsystem interacting with the free-space vacuum. A distinctive feature of the proposed setup is its sensitivity to the relative phase of the applied fields when placed near the plasmonic nanostructure. We demonstrate that due to the presence of the plasmonic nanostructure, the third-order (Kerr-type) susceptibility for one of the laser fields can be significantly modified while another probe field is acting. Moreover, the Kerr nonlinearity of the system can be controlled and even enhanced by varying the distance of the quantum system from the plasmonic nanostructure. We also show that the Kerr nonlinearity of such a system can be controlled by adjusting the relative phase of the applied fields. The results obtained may find potential applications in on-chip nanoscale photonic devices.

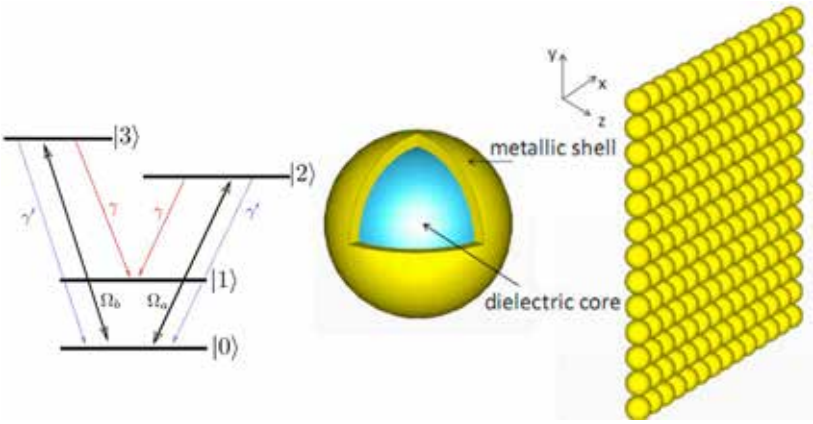

FIG. 1: Schematic diagram of the four-level double-V-type quantum system (left). A metal-coated dielectric nanosphere and a 2D array of such spheres (right).

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Towards a YbF MOT to measure the electron's electric dipole moment

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The excess of matter in the universe cannot be explained by the Standard Model CP-violation, implying the existence of new physics. A measurement of the electron's electric dipole moment (eEDM) exceeding the value predicted by the Standard Model ($< 10^{44}\ e \cdot \mathrm{cm}$) will unveil new CP-violating interactions. The most precise eEDM measurements all use polar molecules, and the current best eEDM limit ($|d_e| < 1.11029\ e \cdot \mathrm{cm}$) was obtained using a beam of ThO molecules [1]. In this experiment, the spin coherence time was about 1 ms. To improve on this, we propose to use ultracold YbF molecules trapped in an optical lattice where spin coherence times of several seconds seem feasible. These molecules have high eEDM sensitivity [2] and can be laser cooled to low temperature [3] so that they can be trapped in a lattice [4].

We will report recent work towards trapping YbF molecules in a magneto-optical trap (MOT). This is significantly more challenging than a MOT for atoms. We use a cryogenic source at 1.8K to form a molecular beam with a mean speed of 50 m/s, a factor 3 slower than previous molecular sources. We are currently working on radiation pressure slowing of the molecules to below 10 m/s, which is the anticipated capture velocity of the MOT. We are also investigating small leaks out of the cooling cycle and how to close them [5].

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Low Energy Electron Attachment to $Co(CO)_3NO$ Clusters

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Interaction of low energy electrons with molecules and molecular clusters is one of the elemental processes in plasma and plasma technologies. In our study we are focusing on electron attachment (EA) and dissociative electron attachment (DEA) on cobalt tricarbonyl nitrosyl ($Co(CO)_3NO$). $Co(CO)_3NO$ is used as a precursor gas for deposition of Co in Focused Electron Beam Induced Deposition (FEBID) and following Electron Beam Induced Surface Activation (EBISA) [1].

Ion yields from our cluster measurements (created by co-expansion with Ar gas) will be compared to previous EA and DEA gas phase $Co(CO)_3NO$ studies [2] and He nanodroplet cluster studies [3]. The gas phase DEA products from Ar clusters agree well with previous works [2,3], comparison with existing gas phase data [2] is shown in Fig. 1 (left). However, formation of cluster products in He nanodroplets [3] and our co-expansion with Ar reveal some differences mostly the shape of the ion yield curves due to the higher energy resolution of the electron beam used in our experiment. The exclusive formation of the molecular ion of $Co(CO)_3NO$ in clusters was confirmed in our measurements but we have detected the ~0 eV resonance for this ion contrary to previous work [3], similarly to other cluster fragments shown in Fig. 1 (right).

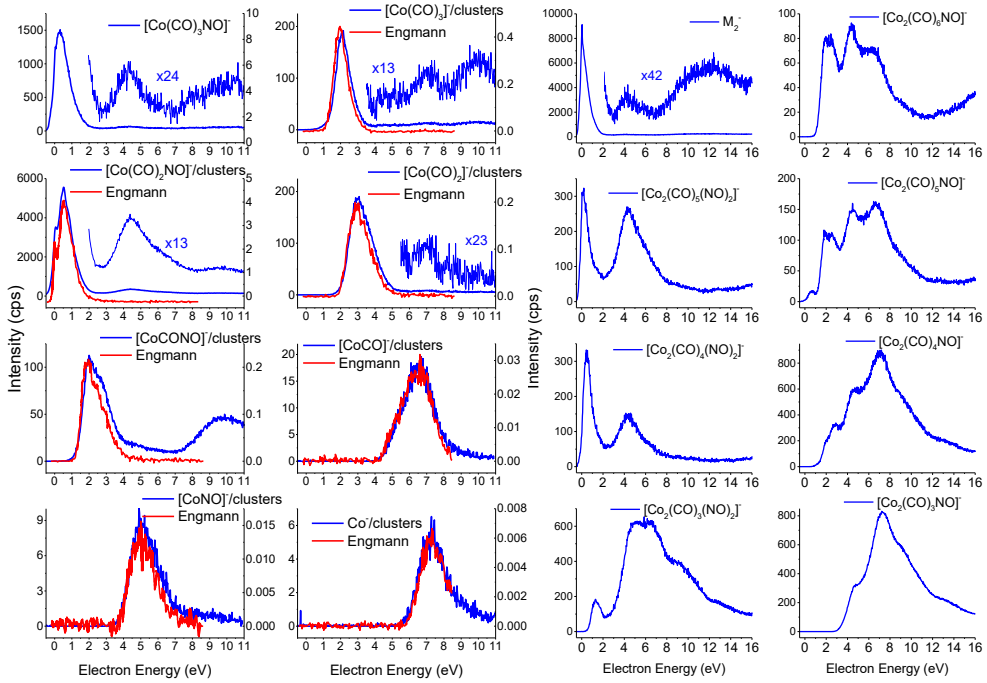

Fig. 1: (left) Comparison of gas phase products from our Ar cluster measurements (blue) with pure gas phase products (red) [2]; (right) Selected cluster fragments from our Ar cluster measurements

This research was supported by Slovak Research and Development Agency project nr. APVV-19-0386 and Grant Agency VEGA project nr. 1/0489/21. This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 692335.

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Cross section analysis in Rayleigh scattering of linearly polarized hard x-rays

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Rayleigh scattering of hard x-rays describes scattering of a photon on an atomic electron without gain or loss of energy. For photon energies below 1 MeV this second order quantum electrodynamical process is the dominant contribution to the elastic scattering of photons on atoms [**1**]. This scattering process can be expressed in terms of the scattering amplitudes $A_{\parallel}$ and $A_{\perp}$ which correspond to the scattering of photons that are linearly polarized in the scattering plane and perpendicular to it, respectively [**2**]. State-of-the-art theoretical calculations of the scattering amplitudes performed within the independent particle approximation predict that the Rayleigh angular distribution strongly depends on the shell structure of the target atom [**3**]. The angular distribution distribution of Rayleigh scattering strongly depends on the (linear) polarization of the incident photon beam [**2**]. Thus a measurement of the angular distribution of scattering a highly linearly polarized photon beam on an atomic target allows for a sensitive test of the underlying theoretical calculations. Modern synchrotron sources which provide hard x-ray beams with a high brilliance that are linearly polarized allow for this kind of experimental investigation. Vice versa, when relying on the theoretical calculations, this scattering process allows for a highly precise determination of the linear polarization of the incident photon beam. While the synchrotron radiation is commonly assumed to be 100% linearly polarized, this is not always the case [**4**]. A measurement of the Rayleigh angular distribution provides for a simple method to determine the actual linear polarization of the synchrotron beam with a high accuracy.

In October 2020 we performed a measurement at the 3rd generation synchrotron source PETRA III at DESY on scattering of a hard x-ray beam ($\hbar\omega = 175$ keV) on a thin gold target. The incident synchrotron beam was linearly polarized in the plane of the synchrotron ring (synchrotron plane). During this experiment the angular scattering distribution was analyzed with a standard Germanium detector positioned within the synchrotron plane and with a 2D sensitive Si(Li) detector positioned both within and out of the synchrotron plane.

Our experimental results show in accordance with theory that the angular distribution of Rayleigh scattering is dominated by scattering on K-shell electrons for large scattering angles while scattering from higher electron shells becomes the dominant contribution when going to forward scattering angles. Including also the data measured for scattering out of the synchrotron plane, we were able to determine the polarization characteristics of the incident synchrotron beam with high accuracy by relying on the theoretical calculations of the scattering amplitudes.

We will present experimental details and first results of this study.

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Experimental Quantum Control on IBM Quantum Computer

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In resonance, pulse shapes have no effect on the population transfer; nevertheless, they affect the resonance response curves of the qubit. In this work, the experimental response curves of various pulse shapes were validated against the theoretical predictions. Furthermore, the effects of symmetrical cropping of the Lorentzian function at different heights were examined, using one of the open-access back-end IBM quantum processors.

Modeling of inter-chlorophyll couplings in the photosynthetic FCP complex

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Photosynthesis has always been one of the most essential processes throughout the development of life on Earth and still has this crucial role today: it allows not only thousands of bacteria, algae and plants to exist but also the codependent animal species to survive. About the same amount of photosynthesis processes are carried out on land and in water, however, it is possible to find photosynthetic organisms in such extremes as deserts or 80 meters deep into the sea [1]. However, one of the most important, but oftentimes forgotten type of photosynthesis–carrying organisms are diatoms – microalgae comprising phytoplankton and accounting for nearly 20 % of global carbon dioxide fixation [2]. Moreover, diatoms have an exceptional light-harvesting complex, fucoxanthin-chlorophyll protein (FCP), which differs from the light-harvesting complex found in higher plants, as it has such chromophores as chlorophyll *c* and fucoxanthin, which guarantee light absorption in the blue-green visible region available in water. Nonetheless, the first crystallographic structure from *Pheodactylum tricornutum* diatom was identified only in 2019 [3], which can allow developing a more thorough theoretical understanding of FCP.

In this study, the Protein Database structure of FCP retrieved from *Phaeodactylum tricornutum* [3] was used to model the first excited state of chlorophylls (Chl) and these results were used to determine their interaction energy. The first excited state of all Chl *a* and *c* pigments was modeled using TD-DFT level of theory with CAM-B3LYP/6-31G(d). The phytyl tail of pigments was cropped as it had very little impact on the transition dipole moment direction and its absolute value. Then transition charge from electrostatic potential (TrEsp) method to calculate transition charges was applied to quantum chemistry calculations results via Multiwfn software [4]. In this work, the CHELPG and MK approaches were used to obtain atomic partial transition charges and subsequently, a consistency check was made, whether it is possible to recreate the $S_0 \longrightarrow S_1$ transition dipole moment. Afterwards, a manual code was written to calculate inter-chlorophyll couplings in the FCP and the results were used for the Förster energy transfer analysis. The Förster energy transfer analysis showed that the strongest interactions between chlorophylls lead to hundreds of femtoseconds – a few picoseconds inverse energy transfer rates and the chlorophyll clusters have an equilibration time of 2 ps. Moreover, these results also indicate a fast energy transfer between chlorophyll *c* and *a*, which is on hundreds of femtoseconds timescale and coincides with previous experimental results.

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The Role of Long-range Pairwise Interactions in Ion-atom-atom Three-body Recombination

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We study the role of the long-range tail of pairwise interactions in ion-atom-atom direct three-body reaction A+A+B$^+$, based on a classical trajectory method in hyperspherical coordinates developed in Ref. [1]. We focus on the formation rate of molecular ions (AB$^+$) and neutral molecules (A$_2$) through this three-body recombination process over a wide range of temperatures. In particular, developing an effective (hyper-) radial potential $V_{\rm eff} \propto \rho^{\beta}$ in hyperspherical coordinates [4], we investigate the previously derived threshold law for ion-neutral-neutral three-body recombination at low temperatures [2,3]. As a result, we explain such threshold law and establish a range for its validity. Furthermore, we find new and intriguing scenarios in which the branching ratio of the product states after three-body recombination deviates from the expected threshold law in the cold regime.

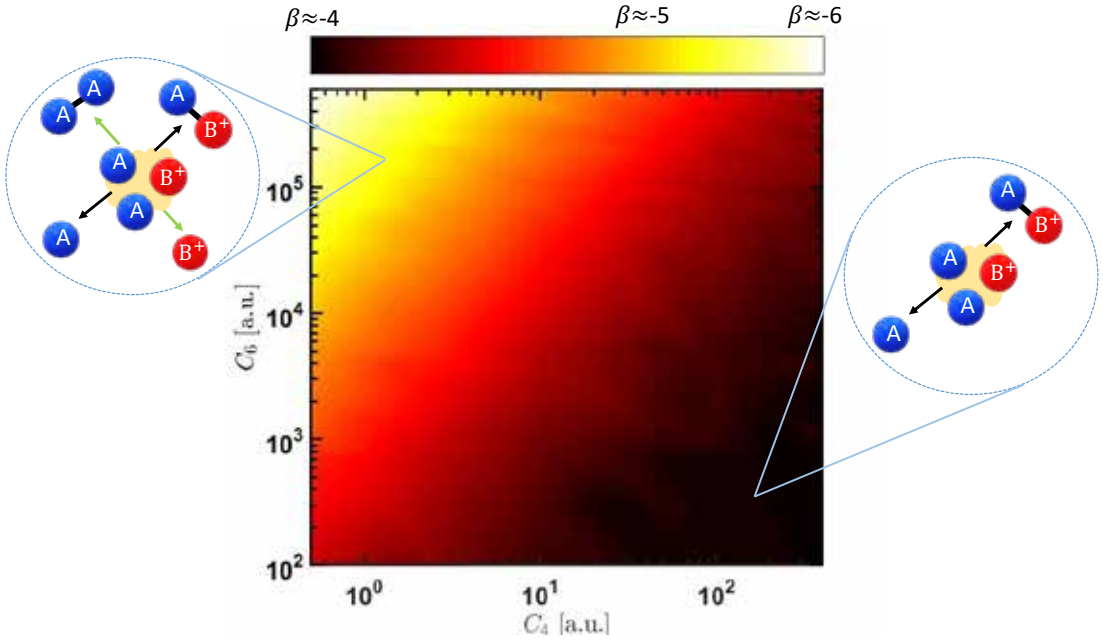

FIG. 1: The power-dependence of the (hyper-) radial potential (β) as a function of coefficients in the long-range two-body interactions $-C_6 r^{-6}$ between two atoms, and $-C_4 r^{-4}$ between ion and atom. The dominant products of the A+A+B$^+$ three-body recombination are shown in the two extreme regimes.

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Floquet soliton formation through periodic driving

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Ultracold atoms are used in optical lattices for quantum simulation of conventionally difficult to computationally simulate many-body systems in condensed matter physics. We present an experimental study of the formation of Floquet solitons from weakly interacting Bose-Einstein condensates of caesium atoms under the influence of a periodically driven optical lattice. Without such periodic driving, matter-waves with zero quasimomentum quickly disperse due to repulsive interactions without the hold of an external trap. With periodic driving, the matter waves are stable and show the dispersionless evolution of a bright soliton, coined as a Floquet soliton. We use the concept of negative effective mass and the resulting changes to the effective trapping potential and interaction strength to explain the stability and time evolution of the wave packets.

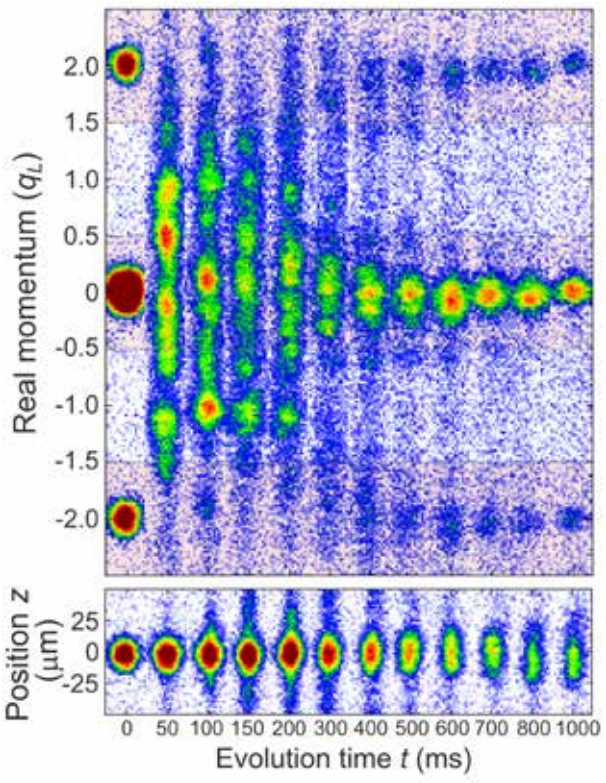

FIG. 1: Formation of a bright Floquet Soliton in momentum space (top) and position space (bottom). The vertical trapping potential is removed at t=0ms and the matter waves freely evolve in the direction of the lattice. The solition forms from 500ms onwards [1].

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Spectroscopy and Dynamics of Flavin Ions in the Gas Phase

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The flavin family of biomolecules is built upon the tricyclic iso-alloxazine moiety. These ubiquitous chromophores perform a wide range of light-dependent reactions in proteins, where micro-environmental interactions may perturb their optical spectra. Flavins are also present in many foods and beverages, which has led to extensive research on the photochemical degradation of flavins in solution. Here there is a history of debate regarding which photoproducts are the result of purely intramolecular processes and which are solvent-assisted or more complex reactions photosensitized by flavins.

We have investigated the intrinsic photochemistry of flavins using gas phase ion luminescnece, photodissociation, and photo-isomerization action spectroscopy, as well as synchrotron photo-electron spectroscopy experiments using an liquid microjet. This work is elucidating the photoprocessing of flavins and is also revealing how the optical spectra of flavins in various charge and redox states are affected by micro-environmental perturbations.

One emerging theme is that non-statistical intramolecular proton transfers between the iso-alloxazine moiety and the phosphoribityl sidechain are dominant photo-induced processes in the gas phase [1, 2, 3, 4]. This leads to the formation flavin derivatives like lumichrome [4] and reduction of the iso-alloxazine chromophore [1], the dominant photoprocesses observed in solution.

The spectroscopy of fully oxidized flavins (structure shown in Figure 1) in the gas phase is found to closely resemble that in solution [1, 2, 3, 4], demonstrating that discrepancies with quantum chemical calculations are not due to solvent effects. Other forms, such as where the iso-alloxazine is deprotonated, exhibit strong charge transfer character and sensitivity to micro-environmental perturbations [3].

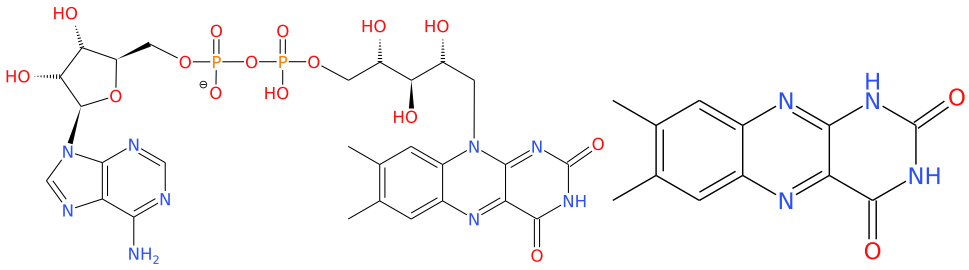

FIG. 1: Structure of fully oxidized Flavin Adenine Dinucleotide mono-anion (left) and its photoproduct lumichrome (right).

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SESSON 3

High resolution molecular spectroscopy in micrometric thin cells

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Shrinking the size of atomic and molecular thin cells is a fascinating prospect with applications for quantum sensing and fundamental physics measurements. Miniature atomic cells were proposed for example as portable atomic clocks and hollow core fibers were filled with molecular gases for applications in frequency referencing [1]. Although compact, the confinement in the above devices remain mesoscopic (larger than the excitation wavelength). Atomic thin cells have been used to probe atoms under sub-wavelength confinement conditions allowing fundamental studies of the Dicke effect [2] and applications in quantum technologies [3]. High resolution probing of sub-wavelength confined molecules is more challenging, due to the small probabilities of molecular transitions, and was so far demonstrated only on a macroscopic cell via selective reflection spectroscopy [4]. Here we extend thin cell platforms to high-resolution molecular spectroscopy. We probe the $\nu 1+\nu 3$ line of acetylene at telecommunication wavelengths ($1.53\mu m$) and SF_6 as well as NH_3 rovibrations at mid-infrared wavelengths ($10.6\mu m$).

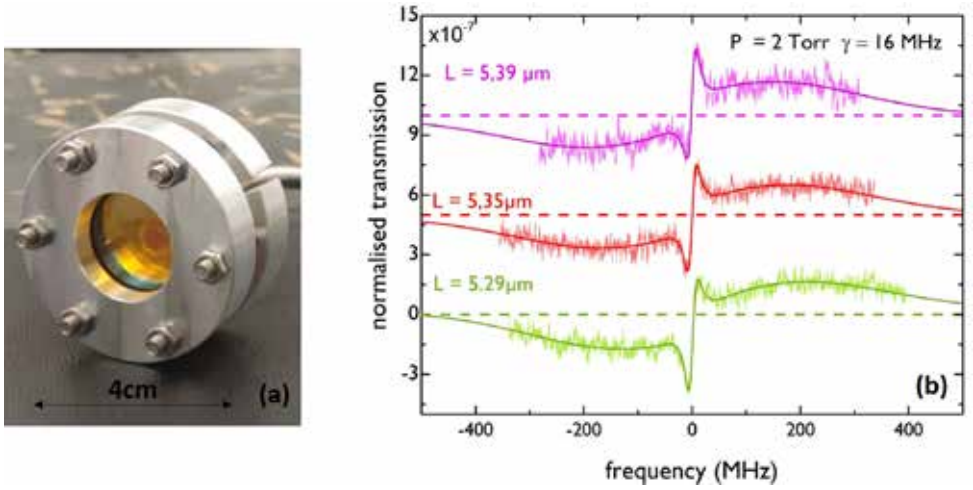

Figure 1: (a) thin cell photograph (b) transmission of an acetylene filled thin cell (2 Torr) at different thicknesses. Theoretical predictions [2] are shown as solid lines. The pressure broadening is 16MHz.

The thin cell was fabricated in our laboratory using ZnSe windows that are transparent through the near and mid infrared spectrum (Fig.1a). The thin cell thickness, measured by Fabry-Perot interferometry, is about $5.35\mu m$ with small variations of about $0.1\mu m$. This cell thickness corresponds to $\lambda/2$ for the SF_6 et NH_3 rovibrations and to $7\lambda/2$ for the combination line of acetylene, conditions for which a Dicke-type narrowing is expected [2]. In our experiments we detect the low power thin-cell optical transmission. A number of techniques were developed to increase the signal to noise ratio and remove the parasitic background from our signals [4]. Our experimental spectra, along with theoretical predictions are shown in Fig.1b. The excellent agreement between theory and experiments suggests that thin cell platforms are very well adapted for compact frequency referencing at telecommunication wavelengths and fundamental physics measurements.

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Spatially Strongly Confined Atomic Excitation via Two Dimensional Stimulated Raman Adiabatic Passage

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We consider a method of sub-wavelength superlocalization and patterning of atomic matter waves via a two dimensional stimulated Raman adiabatic passage (2D STIRAP) [1] process. An atom initially prepared in its ground level interacts with an optical vortex pump beam and a traveling wave Stokes laser beam. The beams are sent in a counter-intuitive temporal sequence, in which the Stokes pulse precedes the pump pulse. The atoms interacting with both the traveling wave and the vortex beam are transferred to a final state through the 2D STIRAP, while those located at the core of the vortex beam remain in the initial state, creating a super-narrow nanometer scale atomic spot. The method allows one to circumvent the restriction set by the diffraction limit inherent to conventional methods for formation of localized solitons, with a full control over the position and size of nanometer resolution defects [2].

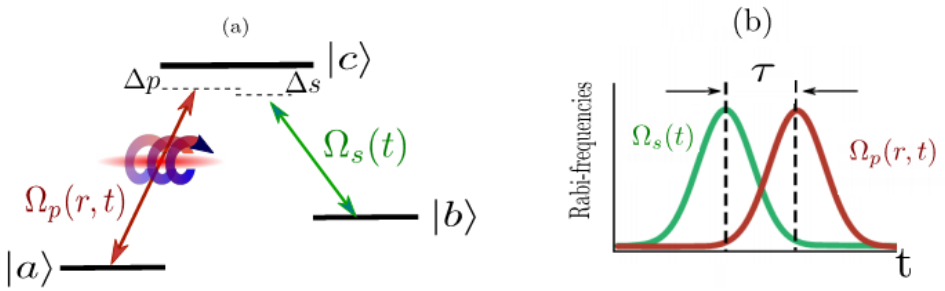

FIG. 1: (a) Schematic representation of a three-level Λ-type atomic system interacting with the pump and Stokes fields characterized by the Rabi-frequencies Ω_p and Ω_s, respectively. (b) Temporal sequence of STIRAP pulses separated by the delay time τ.

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Cusp electron studies in MeV/u collisions of $O^{6+}(1s2s\ ^3S)$ ions with He targets

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The processes of the capture of a target electron into the projectile continuum (ECC) and the loss of a projectile electron into the projectile continuum (ELC) are investigated both experimentally and theoretically for collisions of 24 MeV $O^{6+}(1s2s\ ^3S)$ ions with He gas targets. Double-differential cross sections (DDCS), $d^2\sigma/d\Omega dE$, of the resulting cusp-shaped electron peak were measured at the emission angle of zero degrees with respect to the projectile velocity. The experiments were performed at the NCSR "Demokritos" 5.5 MV Tandem Accelerator Laboratory utilizing an electrostatic single stage hemispherical deflector spectrograph [1]. The cusp electron spectra from the excited $O^{6+}(1s2s\ ^3S)$ state were obtained after applying our double-measurement technique, which requires the same measurement of the cusp peak with O^{6+} projectiles in the ground state ($1s^2\ ^1S$) and with O^{6+} projectiles in the mixed state ($1s^2\ ^1S$, $1s2s\ ^3S$) [2]. Corresponding DDCS calculations, obtained using continuum distorted-wave (CDW) and continuum distorted-wave eikonal initial-state (CDW-EIS) theories [3], are critically compared to the measurements. Our study exposes the role of multi-electron open-shell ions in the dynamics of the ECC and ELC processes providing data that are scarce in the literature.

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S3-P04

The search for Non-IPR isomers of C_{60}^-

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After the accidental discovery of fullerenes [1] and its unequivocally identification in the interstellar medium (ISM) [2], extensive studies were made to elucidate their specific molecular geometries. These were found to be closed cages with an even number of carbon atoms arranged as 12 pentagons and either zero, two or more hexagons. C60 is the smallest member of the fullerene family that obeys the so-called isolated pentagon rule (IPR) [3], where each pentagon is surrounded by 5 hexagons for the most stable isomer. This geometry gives the molecule its exceptional stability and chemical inertness, making it the most abundant of the fullerenes. Every other C60 isomer has at least two pairs of adjacent pentagons. For the most stable non-IPR isomer of the C60- fullerene, the twin adjacent pentagon configuration leads to an enhanced reactivity and a significantly higher electron affinity [4]. This suggests that this isomer could have a significant survival probability and be important for bonding formation processes if formed in e.g. astrophysical environments.

Our pilot studies performed in the cryogenic electrostatic ion storage ring facility DESIREE seems to support this idea. In this storage ring, the spontaneous decay of hot molecules can be followed on timescales up to hundreds of seconds owing to its excellent vacuum conditions (4 cm-3 of residual gas density [5]). The observed decay in the case of C60- at timescales exceeding milliseconds could not be explained by the presence of the IPR isomer alone (Figure 1), which suggests that a small population of the most stable non-IPR isomer of C60-, which do not cool efficiently, is being produced. We aim to further investigate the presence of this isomer by applying laser probing techniques to monitor the depletion of neutral yield as a function of storage time.

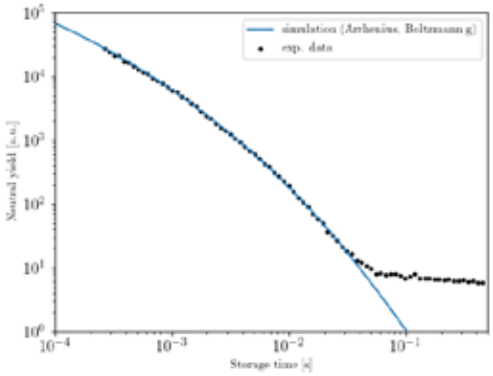

Figure 1. The measured neutral yield as a function of storage time (black data points) due to spontaneous electron emission from internally hot C60-. The solid line shows the results from our master equation simulations of vibrationally assisted detachment (VAD) rates from IPR-fullerenes alone, where the rate is quenched due to efficient radiative cooling processes (recurrent fluorescence) [6]. The measured neutral yield is significantly higher than the model results on timescales exceeding 50 milliseconds, suggesting the presence of non-IPR fullerenes in the ion beam.

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Femtosecond Laser-Induced Low Spatial Frequency Structures On Fused Silica With Tunable-Wavelength Pulses

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Irradiation of inorganic materials with multiple femtosecond laser pulses at high repetition rate induces structural modifications resulting in formation of self-organized laser-induced periodic surface structures (LIPSS) [1]. Many studies of LIPSS predict the dependence of its morphology and periodicity on various experimental parameters such as number of pulses and irradiation wavelength, in particular [2]. The vast majority of experiments were performed mostly by using fundamental wavelengths of standard lasers, so its not enough to fully establish the LIPSS properties in the shortwave infrared range. In this work we present the experimental study of LIPSS morphology and its periodicity in fused silica evolution at high repetition rate with broadly tunable (in the $1-3$ μm range) femtosecond laser pulses.

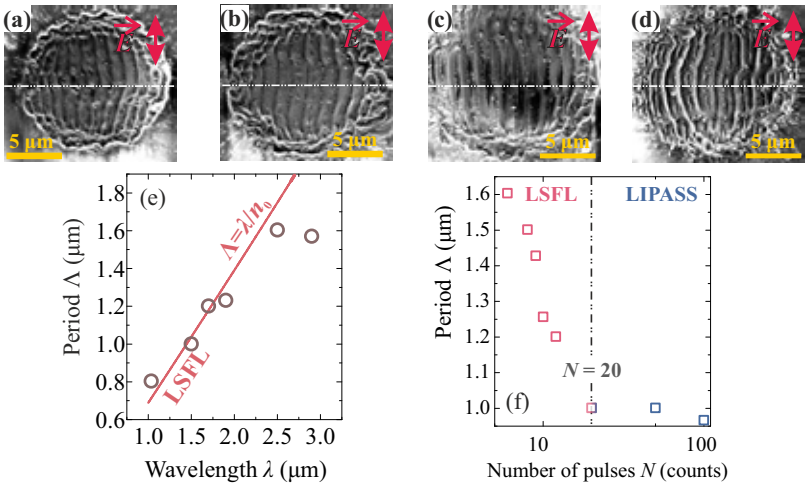

FIG. 1: SEM images of LSFL in fused silica, produced with (a) 1500 nm, (b) 1700 nm, (c) 1900 nm and (d) 2500 nm wavelength pulses. (e) and (f) represent LSFL period dependence on wavelength and number of pulses, respectively.

The experiments were performed using a commercial optical parametric amplifier (Orpheus, Light Conversion Ltd), pumped by Yb:KGW laser pulses, where the pulse duration and repetition rate were 180 fs and 10 kHz, respectively. Fig. 1. (a)–(d) represent SEM images of low-spatial frequency structures (LSFL) in fused silica, produced with different irradiation wavelength pulses and Fig. 1. (e)–(f) show LSFL period evolution with increasing inscription wavelength and number of pulses, respectively. We obtained an increase of LSFL period with increasing the inscription laser wavelength (Fig. 1 (e)), which was also discussed previously for high-spatial frequency structures [3]. In this way, the result indicates the same dependence of period on wavelength for both structures despite different formation mechanisms. Interestingly, we observed that short exposure to laser pulses (Fig. 1. (f)) results in a significant decrease of the period. Such a phenomenon could be caused due to decrease of radiation peak fluence which is governed by surface ablation and formation of a crater.

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Analytical treatment of quantum systems driven by amplitude-modulated time-periodic force using flow equation approach

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Quantum systems driven by external periodic force constitute an immensely practical and, at the same time, quite tractable intermediate case between the two limits of stationary and generic time-dependent systems. Here we will focus on the particular form of the external force, which has a time-periodic part and an additional time-dependent amplitude. The most simplest example can be spin-1/2 particle affected by oscillating magnetic field where the amplitude of the field is not static but additionally performs rotations in space. If oscillation frequency is much larger that the characteristic time of the rotations of the amplitude, then the high-frequency expansion is applicable [1]. Interesting that the effective evolution of such quantum system shows non-Abelian geometric phases.

In order to obtain effective evolution (the evolution averaged over time-periodic oscillation) the main question is to block-diagonalize extended space Hamiltonian. In general it is very difficult task, thus various approximate methods is applicable. One of them is to adapt flow equation approach. Originally the flow equation was proposed by F. Wegner to approximately diagonalize static Hamiltonian [2]. Here we adapt the idea of the flow equation for block-diagonalization and as a consequence to obtain the effective evolution [3]. The advantage of such an approach over previously presented high-frequency expansion is that we can obtain analytical expressions even when the amplitude of the force changes fast (comparable to the high-frequency oscillation), or we can perform automatic derivation of higher order expansion terms using symbolic computational packages.

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Investigation of the molecular-frame photoemission time delay for K-shell photoionization of N_2

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Photoelectron emission time delay (also called Wigner time delay) occurs as a result of the interaction of the emitted photoelectron wave with ionic potential [**1**]. Due to the anisotropic nature of a molecular scattering potential, the Wigner time delay depends on the emission direction of the photoelectron and orientation of the light polarization with respect to the molecular axis [**2**, **3**]. Here, we report Wigner time delays for ionization of $1\sigma_g$, $1\sigma_u$ molecular orbitals (MOs) of N_2 molecule for parallel ($\varepsilon\sigma$-channel) and perpendicular ($\varepsilon\pi$-channel) orientations of the molecule with respect to the electric field vector of linearly polarized ionizing light. As is known [**4**], inter-channel coupling between the partial $1\sigma_g \to \varepsilon\sigma_u$ and $1\sigma_u \to \varepsilon\sigma_g$ photoionization channels leads to an appearance of a $\sigma^\star$-shape resonance in both channels. For these purposes, multichannel single center method was applied to take the inter-channel mixing into account. Moreover, including relaxation of the core (RC), caused by the field of a created core vacancy, yields a correct energy position of the shape resonance [**4**]. Fig. 1 shows the total 1σ-photoemission (average $1\sigma_g$ and $1\sigma_u$ MOs) Wigner time delay of N_2 as a function of the photoelectron kinetic energy and emission angle, computed in coupled-channel relaxed core (CCRC) approximation for the $\varepsilon\sigma$-channel. As one can see from this figure, the total time delay varies in between -10 and $+310$ as. The maximal delay is reached at the position of the shape resonance at about 9 eV [**5**]. With increasing photoelectron energy, the maximal time delay decreases, since a faster electron can easier escape the ionic potential than a slower one. The present theoretical results can be verified by, e.g., a novel experimental approach from [3].

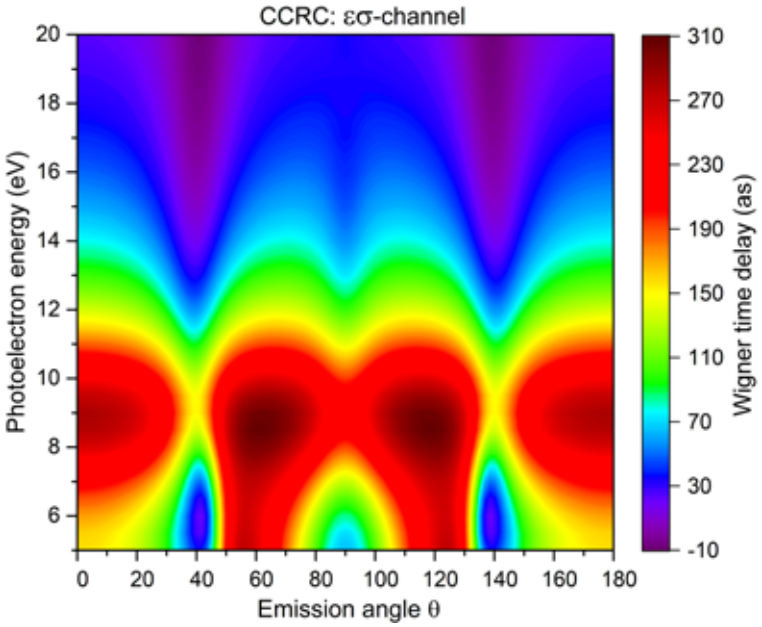

FIG. 1: The total Wigner time delay of N_2 as a function of the photoelectron kinetic energy and emission angle, computed for the $\varepsilon\sigma$-channel.

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Differential Photoelectron Circular Dichroism in Methyloxirane

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The photoelectron circular dichroism (PECD) appears as a forward-backward asymmetry in the laboratory-frame angular distribution of photoelectrons emitted by ionization of chiral molecules with circularly polarized light [**1**]. Most PECD studies are performed in the gas phase for randomly oriented molecules, where this chiral asymmetry reaches a few percent of a total cross section. One of the routes to increase the size of this effect, is to fix a chiral molecule in space [**2**]. As it was shown in [**2**, **3**], fixing one molecular-orientation axis in space can enchance a PECD up to about 20%. In this work, we study experimentally and theoretically the PECD in the fully fixed in space methyloxirane (MOX) molecule, as a function of two molecular orientation angles and two photoelectron emission angles. The experimental data [**4**] were recorded at beam line SEXTANTS of synchrotron SOLEIL, Saint-Abin, France. *Ab initio* calculations were performed by the single center method [**5**]. Fig. 1 depicts experimental (left panel) and theoretical (right panel) differential PECDs for one selected molecular orientation with respect to the light propagation direction. As one can see, the measured differential PECD exceeds 50%, whereas the computed one is somewhat larger and exceeds 80%. Such a strong asymmetry allows to significantly enhance the sensitivity of chiral recognition in the gas-phase.

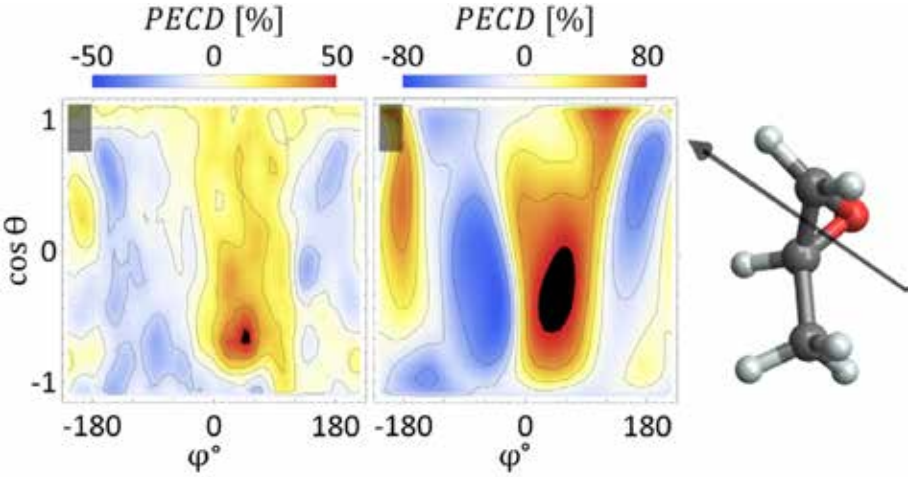

FIG. 1: Measured (left) and computed (right) differential PECDs for S-MOX as functions of the two photoelectron emission (θ, ϕ) angles for selected light propagation direction (see insets).

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Angle-dependent interferences in electron emission accompanying stimulated Compton scattering from molecules

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Kinematically complete synchrotron experiments have recently shown that it is possible to observe Compton scattering of energetic photons from an atomic target with unprecedented detail [1], thus extending the toolbox for investigation of electronic dynamics in atoms and targets. These are very challenging experiments since, beyond the inherent complexity of detecting the resulting charged fragments in coincidence with enough statistics, Compton scattering cross-sections are extremely small (several orders of magnitude smaller than the corresponding photoionization cross section at the same energy). It thus become a formidable challenge to perform the same study on molecules, where the nuclear degrees of freedom must be also accounted for. However, X-ray free electron laser (XFEL) pulses, generated with intensities at least ten orders of magnitude above synchrotron light sources, should be the ideal tool to explore Compton scattering from molecules. The high brilliance of ultrashort X-ray pulses recently generated in free electron lasers already open the way to the investigation of non-linear processes [2] that remained inaccessible over the years due to the smallness of the corresponding cross sections

We present our most recent results on stimulated Compton scattering from fixed-in-space H_2 molecules in the few-hundred eV photon energy range. We employ single pulse [3] and two-pulse schemes [4]. At very high photon energies (above the 1 keV) the dipole approximation is known to fail, and non-dipole corrections terms are required for the proper description of the problem. We extended our previous implementation [5] to include non-dipole corrections ($\mathbf{A}^2$). We here explore the most interesting sub-keV region, where both dipole and non-dipole terms contribute and can eventually become comparable in magnitude. As a result, different quantum paths come into play leading interferences between dipole and non-dipole transitions, which lead to pronounced asymmetries in the electron angular distributions. These asymmetries strongly depend on molecular orientation, to the point that they can lead to electron emission in either the forward or the backward directions with respect to the propagation axis, or in both directions, or even in the orthogonal direction. This is in contrast with Compton scattering from free electrons or atomic targets.

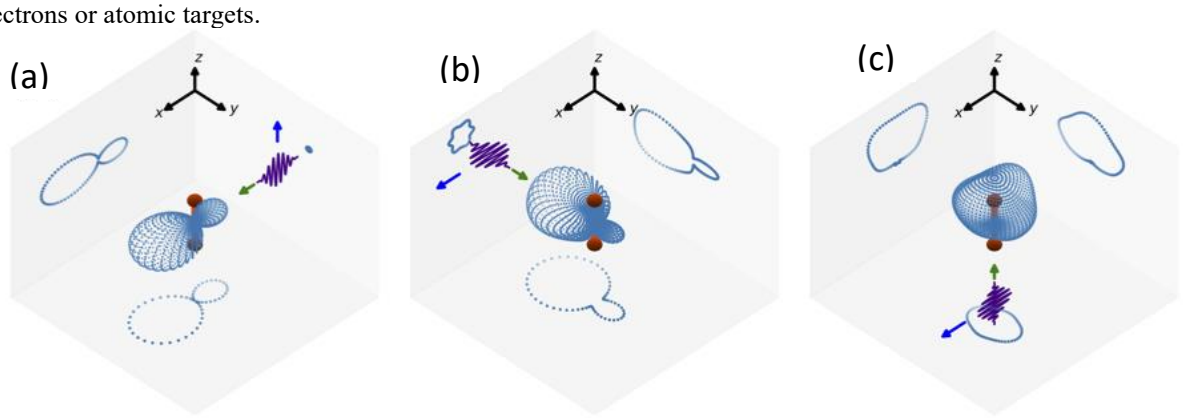

FIG. 1: Molecular-frame photoelectron angular distributions for a single-pulse case. Green arrows: pulse polarization direction. Red arrows: pulse incidence direction. Dark orange spheres: nuclei. Cuts on the xy, xz, and yx planes are also shown. Molecule is along the z axis. a) Polarization along the z axis, incidence direction along the x axis. b) Polarization along the x axis, incidence direction along the y axis. c) Polarization along the x axis, incidence direction along the z axis.

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Relativistic Time-Dependent Configuration Interaction Singles Method

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Attosecond physics aims to unravel the electron motion and coherence in atoms and molecules. Major contributions to this field are the real-time observations of the motion of electrons in ions and atoms through attosecond transient absorption spectroscopy (ATAS) [1,2]. Although the importance of relativistic effects, such as the spin-orbit coupling, was already demonstrated by the first ATAS experiment [1], all ATAS studies have so far been based on non-relativistic theory [3]. Regarding the lack of a relativistic theory, our aim is to develop a general relativistic ATAS method for studying atoms far beyond the perturbative regime [4]. This requires that the N-electron time-dependent Dirac equation is effectively solved. Seeking a compromise between computational cost and accuracy, the relativistic time-dependent configuration interaction singles (RTDCIS) method is proposed [5]. To validate the RTDCIS method, different observables, such as photoionization cross sections, were computed for krypton and xenon, and the results were compared to other relativistic calculations and experimental data (see Figure 1). As expected, the RTDCIS results are similar to the RRPA results within the Tamm-Dancoff approximation (RRPA(TD)). This novel method opens up the possibility to describe the electron spin dynamics by means of spin-resolved ATAS experiments far beyond the perturbative regime. Similarly, it can be applied to other strong-field processes, such as high-order harmonic generation, above-threshold ionization, laser-assisted photoionization, hole alignment, and the study of complex Rabi dynamics.

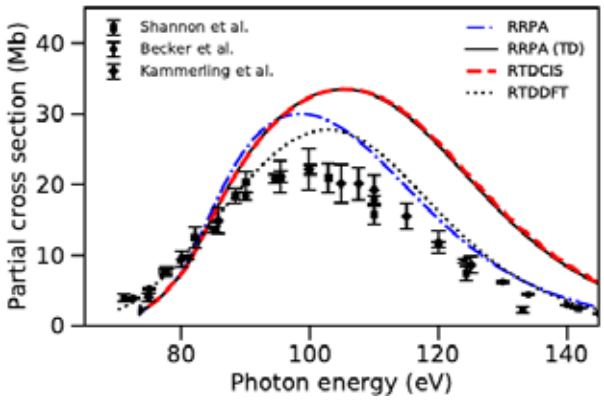

FIG. 1: Xenon partial 4d photoionization cross section. Comparison of different relativistic calculations with experimental results. RTDCIS, RRPA and RRPA(TD) from Ref. [5], RTDDFT from Ref. [6], and experimental data from Refs. [7].

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Superfluid Bose gas on a bubble

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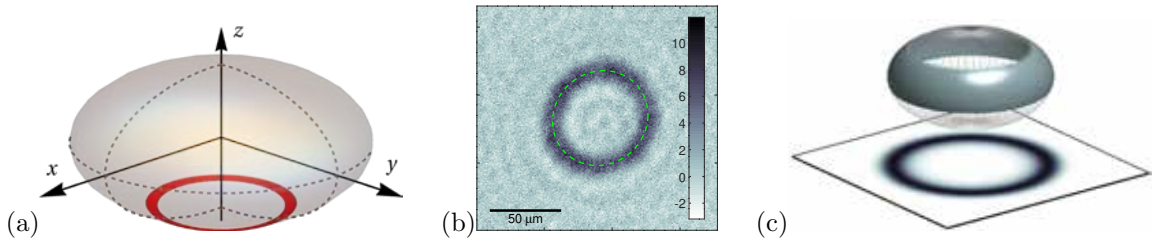
Quantum gases provide us with a very convenient and widely tunable system for the study of superfluidity. In particular, they can be confined in a large variety of geometries (harmonic traps, optical lattices, box traps, lower dimensional traps...), enabling the study of superfluid dynamics with specific contraints. In this work we explore the behaviour of a superfluid quantum gas confined at the surface of an ellipsoid: the atoms can move freely in directions parallel to the surface and are strongly confined in the transverse direction. In a first series of experiments, the atoms initially at rest at the bottom of the shell —because of gravity— are set into rotation: a vortex lattice develops at moderate rotation, and melts for large rotation speeds or low atom numbers. Increasing the rotation further leads to the formation of an annular cloud rotating at supersonic speed, due to the centrifugal force. In a second series of experiment, we implement a way to compensate gravity on the shell. We evidence new effects that prevent the atoms to fill the entire shell, leading again to an annular density distribution but this time in equilibrium.



(a) (b) (c)

FIG. 1: (a) Formation of a superfluid dynamical ring in the bubble trap, and (b) corresponding absorption picture, from the top. (c) Numerical simulation of the spontaneous formation of an annular density in the bubble when gravity is compensated.

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Cavity-based reservoir engineering for periodically driven quantum systems

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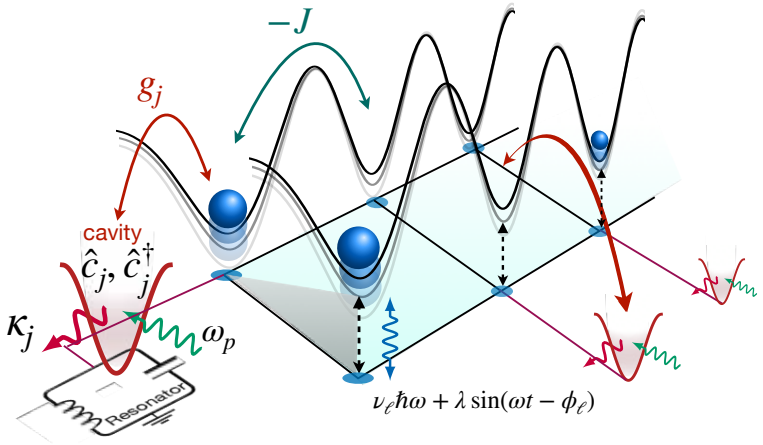
We show that nonequilibrium quantum states can be prepared and stabilized by combining time-periodic driving (Floquet engineering) with synthetic quantum baths, as they can be realized in quantum simulators based on superconducting circuits. Considering lattices of periodically driven artificial atoms coupled to pumped-damped cavities, we characterize regimes, where, on the one hand, the periodic driving can produce effective Hamiltonians with desired properties while, on the other, the cavities induce controlled dissipation cooling the systems to the effective ground state. We will illustrate this mechanism in the robust preparation of non-trivial states such as chiral currents for interacting photons and Aharonov-Bohm cages, where quantum interference constrains the systems to localized states.



Precision Spectroscopy of He-like Uranium Employing Metallic Magnetic Calorimeters

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Recent developments regarding metallic magnetic calorimeters (MMCs) have resulted in a new class of detectors for precision X-ray spectroscopy, for example the maXs detectors [1] (cryogenic micro-calorimeter arrays for high resolution X-ray spectroscopy), which have been developed within the SPARC collaboration. Outstanding features of MMCs are the combination of a very high energy resolution (better than 100 eV FWHM at 100 keV) comparable to crystal spectrometers, with the broad bandwidth acceptance of semiconductor detectors (0.1 – 100 keV) [2]. These detectors are based on the following measurement principle: The energy deposition of an incident X-ray photon leads to a measurable temperature rise of an absorber. At operation temperatures below 50 mK this leads to a change in the magnetisation of a paramagnetic sensor which can be measured by a superconducting quantum interference device (SQUID) [3].

The system is especially well suited for X-ray spectroscopy of highly charged ions, which is a great tool for studying unperturbative quantum electrodynamics (QED) in the regime of extreme electromagnetic fields close to the Schwinger limit. In a recent experiment U^{91+} ions have been stored in CRYRING@ESR at the GSI Helmholtzzentrum für Schwerionenforschung GmbH. Two maXs-type detectors have been deployed at the electron cooler to study the X-ray radiation emitted as a result of recombination events between the electrons and the stored ions. In this contribution we will focus on details of the experimental setup and its integration into the storage ring environment. Noteworthy aspects are a quasi-continuous energy calibration, the truly axial geometry as well as the first exploitation of the time resolution of the maXs detectors to achieve a coincidence measurement with a particle detector.

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Electric-field-controlled dipolar collisions between cold CH_3F molecules in an electrostatic trap

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Polar symmetric-top molecules possess strong long-range dipole-dipole interactions, offering fascinating research opportunities ranging from quantum chemistry to quantum simulation or computation. An essential precondition for these applications is to produce molecular ensembles of high phase-space density. Despite the great progress in recent years in the field of cold and ultracold molecules, this is still an outstanding goal for the desirable class of polar symmetric-top molecules. An established route in the AMO community to increase phase-space density is evaporative cooling, which requires a favorable ratio of thermalizing elastic to inelastic collisions. Therefore, the ability to not only observe collisions between polar symmetric-top molecules but control inelastic collision processes without affecting thermalising elastic collisions is a key step to advance the field further.

In our experiment, we combine cryogenic buffer gas cooling [1] with centrifuge deceleration [2] to confine up to 2×10^7 CH_3F molecules at a density of $10^7/\mathrm{cm}^3$ and a temperature of about 350 mK for several seconds in a microstructured electric trap [3]. This allows us to directly observe cold dipolar collisions between trapped polyatomic molecules with inelastic loss-rate coefficients below 4×10^{-8} cm^3/s. We control the latter by utilizing a homogeneous control field that covers a large fraction of the trap volume. Excellent agreement between experimental data and a semi-classical model is observed, which allows us to identify the dominant loss mechanism ($\sim 95\%$) to be dipolar relaxation [4] to untrapped rotational states. In conclusion, we demonstrate the suppression of inelastic collisional losses by more than a factor of two using an external electric field. This controllability can be an important tool for future rethermalisation or evaporative cooling experiments.

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Relativistic Inelastic Electron Scattering on Atoms and Ions; Calculations of Total Cross Sections and Collision Strengths in GRASP - Description of the Method

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Total cross sections and collision strengths are parameters that describe the behaviour of an atom or ion when it is bombarded by other particles ie. electrons. Inelastic scattering describes such collisions in which the state of a target is changed. To describe also the change of the spin of an electron, a relativistic approach must be applied. Relativistic inelastic electron scattering can be observed in kilonovae and supernovae, hence total cross sections and collisions strengths are used in astrophysics [1].

In atomic and particle physics there are two common methods of calculating cross sections. The first one revolves around the Lippmann-Schwinger equation and is using Green functions [2]. The second one is a popular R-matrix method [3].

In our method, the multi-configuration self-consistent-field Dirac-Hartree-Fock (MCSCF DHF) method is used to calculate numerical representations of target state wavefunctions. Then they are used in the relativistic close-coupling equations

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}+\frac{\kappa}{r}\right)P_{k,\kappa\epsilon}(r)-\left(2c+\frac{\epsilon}{c}\right)Q_{k,\kappa\epsilon}(r)=-\frac{1}{c}\sum_j(V_{kj}(r)+K_{kj}(r))Q_{j,\kappa\epsilon}(r) \tag{1}$$

$$\left(\frac{\mathrm{d}}{\mathrm{d}r}-\frac{\kappa}{r}\right)Q_{k,\kappa\epsilon}(r)+\frac{\epsilon}{c}P_{k,\kappa\epsilon}(r)=\frac{1}{c}\sum_j(V_{kj}(r)+K_{kj}(r))P_{j,\kappa\epsilon}(r) \tag{2}$$

where V_{kj} and K_{kj} are respectively Coulomb and exchange potentials.

These equations then can be integrated outward to obtain radial continuum wavefunctions, from which the total cross section can be obtained. Similar calculations in the elastic case have been done [4] and a first attempt at the method has been presented but not developed [5].
All calculations are done in GRASP2018 [6] and a new subprogramme will be implemented to GRASP to enable these calculations to other research groups. Work is in progress and we expect to present preliminary numerical results.

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One-axis twisting as a method of generating many-body Bell correlations

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We demonstrate that the one-axis twisting (OAT), a versatile method of creating non-classical states of bosonic qubits, is a powerful source of many-body Bell correlations. We develop a fully analytical and universal treatment of the process, which allows to identify the critical time at which the Bell correlations emerge, and predict the depth of Bell correlations at all subsequent times [**1**].

Next, our findings are illustrated with a highly non-trivial example of the OAT dynamics generated using the two-component Bose-Hubbard model realized in a system composed by a few ultracold atoms trapped in a one-dimensional optical lattice. The system, initially in the superfluid phase with each atom in a superposition of two internal states, is first dynamically entangled by atom-atom interactions and then adiabatically brought to the Mott-insulator phase with one atom per site where the quantum correlations are stored [**2**].

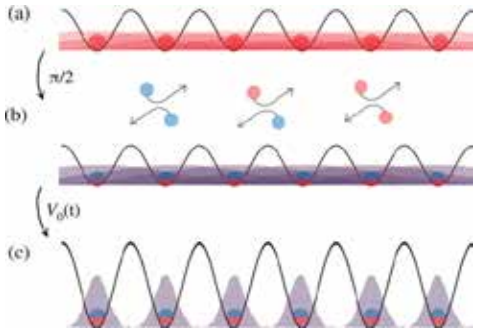

Figure 1: (a) Initially, ultracold atoms in an internal state a are prepared in the superfluid phase in a shallow optical lattice with unit filling. (b) At time $t = 0$, a $\pi/2$ pulse puts each atom in a coherent superposition of two internal states a and b. Immediately after the pulse, while the system is in the superfluid phase, binary atomic interactions between atoms starts the generation of quantum correlations in the system. (c) The lattice height is gradually increased in such a way that the system undergoes the Mott-insulator transition with one atom per site at the "best time" to store in the lattice either the best squeezing or a GHZ state.

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One-axis twisting as a method of generating many-body Bell correlations
Work under preparation

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Producing and storing spin-squeezed states and Greenberger-Horne-Zeilinger states in a one-dimensional optical lattice
Phys. Rev. A, **102**, 013328 (2020)

Isosteric molecules in the time-domain

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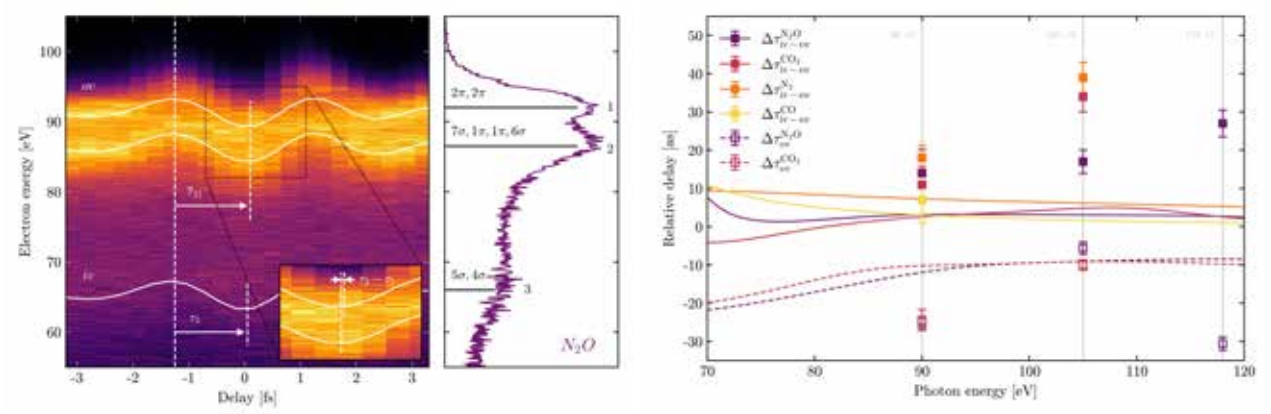
In this work, we report on photoemission timing measurements performed on small isosteric molecules on an attosecond timescale in the gas phase. By comparing the photoemission time delay between the respective σ and π orbitals in the inner (iv) and outer (ov) valence states of CO_2 and N_2O we expect to find deeper insight into the characteristics of isosterism in the time-domain. Furthermore, the isoelectronicity of CO and N_2 is investigated in detail as a complementary study. Due to the similarities in molecular structure (isostericity) and electronic configurations (isoelectronicity) the pure effect of the specific molecular/orbital characteristics is expected to be probed. The results regarding similarities and differences in photoemission dynamics can serve as a stepping stone for isosteric characteristics in these molecules and may bear the potential to draw conclusions from these simple systems to unknown or unexplored isosteric molecular bonds in general. The measurement campaign so far provided interband ($\Delta\tau_{\mathrm{iv-ov}}$) as well as intraband ($\Delta\tau_{\mathrm{ov}}$) relative photoemission time delays for N_2O, CO_2, N_2 and CO via attosecond streaking spectroscopy. Exemplary for all molecules, the figure on the left shows the streaking trace for N_2O together with its static spectrum and the marked orbital groups for extracting the inter- and intraband delays [**1**].



Scattering calculations help us to gain a greater understanding of the correlations between molecular geometry and photoemission time and therefore the isosteric influence, with the focus on assessing the differences between modelling and experimental findings. The figure on the right shows the corresponding ePolyScat [**2**, **3**, **4**, **5**] calculation results (solid and dashed lines) together with the extracted delays from the streaking measurements (squares) via diffrTDSE [**6**]. The experimental data show great correspondence and consistency but also overall deviations from the calculated expected values, which are determined but not completely understood up to now. As the calculations are only taking the Eisenbud Wigner-Smith delay and the addition of the laser induced Coulomb-laser coupling delay contribution into account, the aim is to determine the missing further delay contribution. Absolute photoemission timing via the atomic chronoscope method [**1**] in order to gain a deeper insight into the isosteric/isoelectronic comparability in the time-domain together with the verification of a relation to Yijie Liao et.al's [**7**] findings of an photon energy dependent oscillation in the photoemission time delay of asymmetric molecules are two further steps on the path of completing the picture.

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Ultra-Stable, Continuous-Wave Light Source for ^{114}Cd and ^{174}Yb Atomic absorption line measurement for Precision Thermometry

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We present a highly stable ultraviolet (UV) and visible light sources for primary high-temperature Doppler broadening thermometry (DBT) close to the freezing points of Sn at 505 K (232˚C) and Zn at 693 K (420˚C), which are defining fixed point of the International Temperature Scale of 1990 (ITS-90). The main goal of this research is to lower the uncertainty in the fixed points in use today and to take a step toward primary thermometry without fixed points and interpolation. Accurate recording of the absorption of ^{114}Cd and ^{174}Yb as a function of frequency at low pressure links the thermal energy of the vapour to frequency [1,2], which is the physical quantity that can be measured the most accurately. Table 1 shows the resonance transition wavelength, Doppler broadened linewidth, natural linewidth, absorption coefficient at room temperature, vapour pressure, and temperature T required to obtain a vapour pressure giving the absorption coefficient of 1 cm^{-1}.

	λ (nm)	Doppler (MHz)	Natural (kHz)	α 298K (cm^{-1})	P(mbar)	T (K)
^{114} Cd	326.2	1411	65	1e-8	7e-3	523
^{174}Yb	555.8	751	180	1e-14	5e-4	658

Table 1: Properties of ^{114}Cd and ^{174}Yb vapour absorption lines at 326.2 nm and 555.8 nm [3].

Figure 1 shows a schematic of the optical setup for ^{114}Cd and ^{174}Yb absorption line measurements. Pump light is generated at 652.4 nm by sum frequency generation (SFG) of two IR lasers at 1579 nm and 1112 nm. Both lasers are phase locked to a frequency comb that is in turn phase locked to an ultra-stable laser. UV light at 326.2 nm is then produced via second harmonic generation (SHG) in a β-BaB_2O_4 (BBO) crystal in a bow-tie cavity (Agile Optic GmbH) [4]. The power stability, linewidth, and continuous tuning range of the UV light is studied. Cavity length is stabilized to the pump wavelength at 652.4 nm using the Hänsch-Coulliaud locking technique [5]. A silicon carbide (SiC) photodiode [6] is used to measure the absorption line at 326.2 nm. For ^{174}Yb absorption line measurement a probe light at 555.8nm is generated using SHG of the 1111.6 nm using a Magnesium-doped Periodically Poled Lithium Niobate crystal (MgO:PPLN). Transmission through both vapour cells is measured as the probe laser frequency scans about 20 GHz across both atomic absorption lines of ^{114}Cd and ^{174}Yb. The optical power is actively stabilized via an acousto-optical modulator (AOM) before entering the vapour cells.

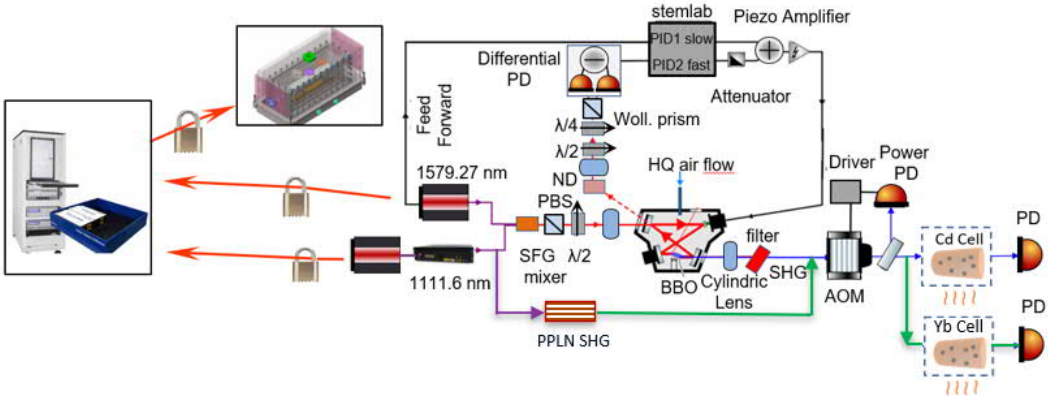

FIG. 1: Schematic overview of the experimental setup for UV light generation at 326.2 nm for ^{114}Cd (blue beam line) and visible light generation at 555.8 nm for ^{174}Yb (green beam line) absorption line measurements.

Experimental set up in Fig. 1 is designed with the capability to be modified for the absorption line measurement of ^{64}Zn at 307.7 nm. In the case of ^{64}Zn, 615.4 nm light is generated from IR lasers at 1111.6 nm and 1378.6 nm via SFG. The same SHG cavity optics is suitable for the generation of UV light at 307.7nm accessible with BBO.

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The Correlation in Three-Electron Dynamics in a Strong-Field Ionization

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Multiple non-sequential ionization is an excellent example of correlations. Thanks to recent advances in theoretical methodology, it became possible to construct a model that allows quantum-mechanical studies on triple ionization [1]. As a result [1-3], the influence of the symmetry of the initial wave function on ionization yields was investigated and the correlated dynamics was confirmed on Dalitz plots, called ternary spectra. However, the analysis of these spectra was seriously limited, since it is not a trivial task to separate the different ionization paths in quantum-mechanical modelling. In the following, using the classical-trajectory Monte Carlo method, we model the interaction of the three-electron atom with a strong, linearly polarized laser field [4]. The final electron momenta distributions are again visualized with Dalitz plots. This time, we identify the traces of particular ionization paths in these spectra and demonstrate that by analyzing Dalitz plots even the information on the relative role of various channels may be retrieved. Using the same method, we show that it is possible to differentiate the multi-recollision events from other channels. We suggest that Dalitz plots are a convenient tool for studying non-sequential triple ionization [5].

This work was supported by Innovation Program of Shanghai Municipal Education Commission (2017-01-07-00- 02-E00034), National Key R&D Program of China (2018YFA0404802), National Natural Science Foundation of China (NSFC) (Grants No. 11925405 and No. 91850203). The simulations were performed on the π supercomputer at Shanghai Jiao Tong University. This work was realized under National Science Centre (Poland) project Symfonia No. 270 2016/20/W/ST4/00314.

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Accuracy of allowed and forbidden transition properties for atoms/ions in Sb-isoelectronic sequence

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We aim to investigate atomic properties of Sb-like isoelectronic sequence: Sb I, Te II, I III, Xe IV, and Cs V. The multiconfiguration Dirac-Hartree-Fock and relativistic configuration interaction methods, which are implemented in the general-purpose relativistic atomic structure package GRASP2018 [1], are used in the present work. We computed the lowest energy levels of the $5s^25p^3$, $5s5p^4$, $5s5p^35d$, and $5s^25p^2\{6s, 7s, 6p, 7p, 5d, 6d, 4f\}$ configurations, allowed (E1) and forbidden (M1,E2) transitions between levels of these configurations. Core-core, core-valence correlations are investigated in the relativistic configuration interaction computations.

Table 1: Mean energy differences (in cm^{-1}) from the NIST ASD and mean relative differences are given in parentheses (in %) for the Sb I-Cs V.

	Sb I	Te II	I III	Xe IV	Cs V
$5s^25p^3$	660(5.3)	399(2.7)	611(3.4)	455(2.3)	739(2.8)
$5s5p^4$	(-)	1302(1.6)	1600(1.4)	1625(1.2)	1542(0.9)
$5s^25p^26s$	394(0.7)	200(0.2)	1054(0.8)	1426(0.8)	2591(1.1)
$5s^25p^27s$	427(0.7)	382(0.7)	209(0.1)	...(...)	...(...)
$5s^25p^26p$	233(0.4)	298(0.3)	...(...)	1041(0.5)	...(...)
$5s^25p^27p$	512(0.8)	801(0.6)	...(...)	...(...)	...(...)
$5s^25p^25d$	297(0.5)	510(0.5)	1365(1.0)	1862(1.1)	3594(1.8)
$5s^25p^26d$	799(1.2)	419(0.3)	416(0.2)	...(...)	...(...)
$5s^25p^24f$	169(0.3)	536(0.4)	...(...)	6411(3.2)	...(...)
All	412(0.9)	415(0.6)	892(0.8)	2708(1.5)	2452(1.4)

Accuracy of energy levels are evaluated by comparing it with the National Institute of Standards and Technology Atomic Spectra Database (NIST ASD) [2] recommended values and with other methods. Mean differences and mean relative differences (averaged over the levels in the configurations) are given for all investigated elements in Table 1. A lot of levels are missing in the NIST ASD. Accuracy estimation for line strengths of E1- and E2-type transitions is described in [3]. This estimation is based on line strengths dependence on gauge. More about transition properties and it's accuracy for all investigated atoms/ions will be presented during the conference.

Acknowledgements: This project has received funding from European Social Fund (project No 09.3.3-LMT-K-712-19-0080) under grant agreement with the Research Council of Lithuania (LMTLT).

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Engineering spin dynamics in a superradiant quantum gas

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Dynamic transients are a natural ingredient of non-equilibrium quantum systems. One paradigmatic example is Dicke superradiance, describing the collectively enhanced population inversion of an ensemble of two-level atoms coupled to a single mode of light. We present a new experimental approach, which exploits superradiance in a quantum degenerate gas to engineer dynamical tunneling in a synthetic lattice geometry.

Our experimental implementation is based on a spinor Bose-Einstein condensate which is coupled to a single mode of an ultrahigh-finesse optical cavity [**1, 2**]. Transverse laser fields induce cavity-assisted Raman transitions between discrete momentum states of two spin levels, which we interpret as tunnelling in a momentum-space lattice. As the cavity field depends on the local density and spin configuration, the tunneling rate evolves dynamically with the atomic state. By monitoring the cavity leakage, we gain real-time access to the emerging currents and benchmark their collective behaviour.

As an extension, by detuning the drive far from two-photon Raman resonance, we can engineer higher-order processes that can be described by effective spin-spin interactions mediated by the cavity. By coupling spin and momentum we directly observe this effect which can manifest itself both as a pair production or as a spin-exchange process. Our results provide prospects to implement dynamical gauge fields and fast entanglement dynamics far from equilibrium.

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Towards sympathetic cooling of laser-cooled molecules with ultracold atoms

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Ultracold molecules have a diverse range of potential applications including tests of fundamental physics, quantum information processing, and quantum chemistry [1]. For all of these applications it is beneficial to have access to samples of molecules with high phase space density, even up to quantum degeneracy. This is a particular challenge for laser-cooled molecules - although advanced techniques have allowed cooling down to a few µK [2, 3], it seems unfeasible that much lower temperatures will be reached with direct methods. Moreover, the densities of laser-cooled molecules currently available are insufficient for evaporative cooling to be effective. A possible way to bypass this problem is through sympathetic cooling with ultracold atoms [4].

For sympathetic cooling to work effectively, the rate of elastic collisions between the molecules and atoms must be larger than the loss rate due to inelastic collisions. In our previous work [5], we measured the loss of laser-cooled CaF molecules due to inelastic collisions with ultracold Rb atoms in a magnetic trap and identified a molecular state in which this loss was greatly suppressed. Building upon this, we were able to put an upper bound on the elastic collision cross section between the two species but further measurements were limited by the density of molecules in the trap.

In this work, we present our progress in increasing the number of trapped molecules by implementing transverse cooling and improved optical pumping. For our previous experiments, a cold beam of CaF molecules was created in a cryogenic buffer gas source before being loaded into a magneto-optical trap (MOT). Due to the spread of transverse velocities in the beam, only a small fraction of the molecules produced by the source reached the MOT. Our newly applied transverse cooling increases the number of molecules captured by reducing the divergence of the beam. From the MOT, our new optical pumping scheme directly prepares the molecules in a magnetically trappable state, increasing the loading efficiency into the magnetic trap. With both these improvements, we can increase the density of molecules in the magnetic trap by a factor of 7 compared with our previous work.

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S3-P23

Investigation of intramolecular charge transfer with non-linear X-Ray spectroscopy: theoretical challenges in the description of coherent wave-packets and their properties

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In complex chemical processes such as photosynthesis and cellular respiration, a pivotal role is played by intramolecular charge transfer reactions (ICT). The understanding of ICT on the microscopic level would give a decisive contribution to the comprehension of these very efficient natural processes and potentially allow for applications in important fields like solar cells and molecular electronics [**1**][**2**].
ICT consists of the transfer of charge through the covalently bonded structure of a molecule. On the microscopic level this corresponds to the time evolution of a wave-packet, which coherently evolves as charge is transferred. The advent of X-Ray Free Electron Lasers (XFEL), with their capability of delivering very intense attosecond pulses, opens to the application of non-linear X-Ray spectroscopic techniques to the study of ultrafast chemical reactions such as ICT. In particular, Stimulated Resonant Inelastic X-Ray Scattering (SRIXS), is a promising non-linear spectroscopic technique, capable of launching a coherent vibronic wave-packet of valence excited states from a specific element of a molecule [**3**]. This allows for both time and spatially resolved studies of ICT.
The theoretical description of a molecular wave-packet and its time propagation, requires both an accurate theory of light-matter interaction and a precise quantum-chemical treatment of the molecular states involved. In this presentation, a theory for the description of a SRIXS wave-packet and its time propagation will be presented. While the light matter-interaction is treated by means of time-dependent perturbation theory, the Equation of motion Coupled Cluster method (EOM-CC) is used for the description of the molecular states and their properties. The EOM-CC method is considered the state-of-the-art in X-Ray spectroscopy calculations, and it is often used as the reference in benchmark studies [**4**]. Despite its high accuracy, EOM-CC is based on non-adjoint excitation operators which leads to a non-hermitian representation of the density matrix of the wave-packet. Consequently, properties depending on the populations of the density matrix are well defined, while the ones depending on the coherences are not. This poses challenges in the design and the accurate calculation of observables describing the coherent wave-packet. This presentation will discuss the implementation and the challenges connected with it, while highlighting the open issues and discussing possible developments.

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Ion Trap Study of the Isotope Exchange in Collisions of OH^- and OD^- with HD at Temperatures down to 10 K.

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In the past twenty years, the OH^- and OD^- anions have been the subject of numerous theoretical and experimental studies, which investigated, e.g., their formation and destruction in various environments, their rotational spectra with high precision, or their presence in the interstellar medium (see Ref. [2] and references therein).

This work presents the rate coefficients of the following astrochemically relevant isotope exchange reactions

$$OH^- + HD \xrightarrow{k_1} OD^- + H_2, \qquad \Delta H^0 = -24 \text{ meV}, \tag{1}$$

$$OD^- + HD \xrightarrow{k_2} OH^- + D_2, \qquad \Delta H^0 = 17 \text{ meV} \tag{2}$$

at temperatures between 10 and 300 K. The measurements were carried in a cryogenic radiofrequency 22-pole trap. This is a follow-up to our previous studies of the reverse reactions [1, 2]

$$OD^- + H_2 \xrightarrow{k_{1r}} OH^- + HD, \qquad \Delta H^0 = 24 \text{ meV}, \tag{3}$$

$$OH^- + D_2 \xrightarrow{k_{2r}} OD^- + HD, \qquad \Delta H^0 = -17 \text{ meV}. \tag{4}$$

The knowledge of the forward and reverse reaction rate coefficients allows us to evaluate the equilibrium constants of these reactions and consequently to validate the theoretical reaction endothermicities ΔH^0 at 0 K given above.

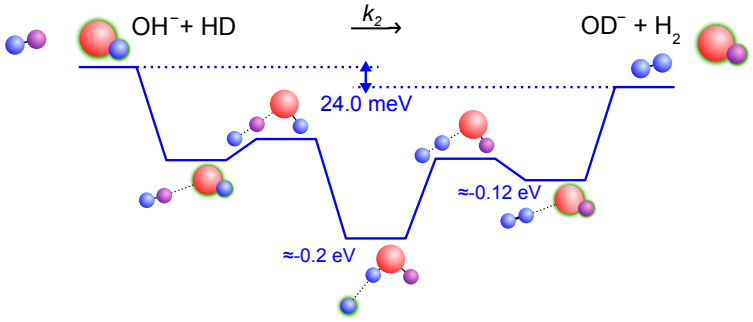

FIG. 1: Schematic view of the OH^- + HD reaction path. Adopted from [1]. See [1] for detailed explanation.

This work was supported by the Czech Science Foundation projects 20-22000S and 21-28560S and Charles University Grant Agency 37672.

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Theoretical study of energy spectra and radiative transitions of Pr^{3+} ion

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In the past years the interest of heavy elements, especially of the lanthanide elements, was increased when gravitational waves from the neutron star merger GW170817 and its electromagnetic counterpart (AT2017gfo) were observed. The observed properties of AT2017gfo at ultraviolet, optical, and infrared wavelengths are found to be consistent with theoretically expected "kilonova". To firmly identify the heavy elements in kilonova spectra, accurate and complete atomic data are necessary.

In the present work, energy spectra computations using GRASP2018 [1] code were performed for the 1110 levels (up to the 32.3 eV energy limit). The levels of the inner-shell-excited configurations ($5p^5\{4f^3, 4f^25d, 4f^26s, 4f^26p, 4f5d^2\}$) were also studied. To evaluate the accuracy of the results, the calculated energy levels were compared with data from the Atomic Spectra Database (ASD) of the National Institute of Standards and Technology (NIST) [2] (see Figure 1). In the figure, energy levels belonging to different configurations are distinguished. The agreement for the levels of the same configuration is similar, except the ground configuration. The first six levels of the ground configuration agree with NIST ASD recommended values within 500 cm^{-1}. The differences for the remaining levels of this configuration reaches 2500 cm^{-1}. There is good agreement for the present energy levels of the low excited configurations, the differences for the levels of the $5p^64f5d$, $5p^64f6s$, $5p^64f6p$ configurations reaches 1000 cm^{-1}. The larger disagreement (differences up to 4000 cm^{-1}) is for the levels of the $5p^64f6d$, $5p^64f7s$, $5p^64f5f$ configurations.

Transition data of electric dipole (E1) transitions are calculated between the all obtained levels. The uncertainties of the E1 line strengths are estimated based on the methodology described in [3].

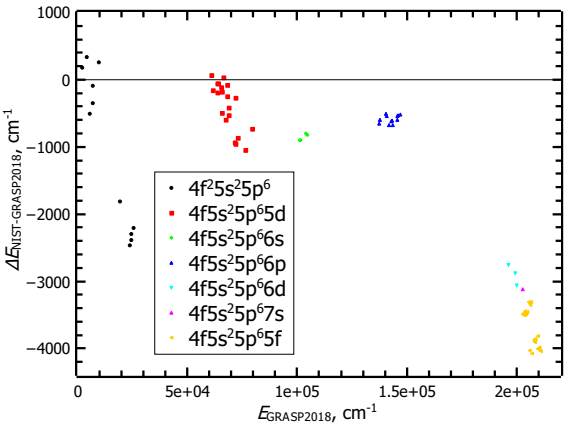

FIG. 1: Differences between NIST ASD energy levels and those of the present GRASP2018 calculations.

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Condensed matter in big time crystals at room temperature

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Big discrete time crystals consist of many unit cells in the time dimension similarly like ordinary space crystals possess many unit cells in space [1]. Condensed matter phenomena can be realized in big time crystals only. We describe condensed matter physics in the time dimension and report experimental demonstration of big discrete time crystals in an optical system at room temperature [2]. The experiments constitute a milestone towards chip-scale time crystals, paving the way from complex labs toward real-world applications.

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New Discoveries About Photon

Given that the birthplace of photon is the electron and the photons emit from the electrons and continue on their trajectory, in fact, the trajectory of each photon depends on the type of motion of the electron in which is transferred to photon. Electrons usually have two main motions; the first one is around the nucleus and the other one is around themselves. On the other hand, the photon also has a rotational motion around itself. When a photon emits from an electron, its motion is the resultant of these three types of motions. Photon obtains its wavelength from the motion of electron around the nucleus. The combination of the rotational motion of electron around itself and the rotational motion of photon around itself creates a zigzag-like motion in a closed ring, which can be called the internal motion of the photon.

In this paper, by using this type of motion for the photon, as well as considering a photon as a particle with a constant mass, we will express the photon energy equation and we are going to define the nature of superstrings and structure of subatomic particles.

Quasi-BIC mode lasing in a quadrumer plasmonic lattice

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Plasmonic lattices of metal nanoparticles have emerged as an effective platform for strong light-matter coupling, lasing, and Bose-Einstein condensation. However, the full potential of complex unit cell structures has not been ex- ploited. On the other hand, bound states in continuum (BICs) have attracted attention, as they provide topologically protected optical modes with diverging quality factors. Here, we show that quadrumer nanoparticle lattices enable lasing in a quasi-BIC mode with a highly out-of-plane character. By combining theory with polarization-resolved measurements of the emission, we show that the lasing mode has a topological charge. Our analysis reveals that the mode is primarily polarized out-of-plane as a result of the quadrumer structure. The quality factors of the out-of-plane BIC modes of the quadrumer array can be exceedingly high. Our results unveil the power of complex multi-particle unit cells in creating topologically protected high-Q modes in periodic nanostructures.

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High-precision determination of the atomic mass of Helium-4 and other light atomic nuclei

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Atomic masses with high precision can be obtained by Penning-trap mass spectrometry. The LIONTRAP experiment is one such high-precision mass spectrometer that can achieve relative mass uncertainties of the order of 10^{-11} and is dedicated to light ions. The results at LIONTRAP include the atomic mass measurements of the proton [1], the deuteron and the HD^+ molecular ion [2]. The deuteron mass was measured to a relative precision of 8.5 ppt [2]. Our results show an excellent agreement with values that were extracted from laser spectroscopy of HD^+ [3]. This comparison is currently limited by the precision of the electron's mass in atomic mass units (amu), derived from a measurement of the bound electron g-factor in $^{12}C^{5+}$ [4]. ^{4}He is a prime candidate for a future improvement, as it is far less sensitive to higher-order terms of quantum electrodynamics (QED) and to the charge radius of the nucleus. Currently, we are measuring the atomic mass of ^{4}He to support such a determination of the electron mass in amu. Furthermore, the mass difference of T and ^{3}He nuclei, measured with the highest precision, will allow an important consistency check for the systematic uncertainty of an upper limit of the $m(\bar{\nu_e})$ by the KATRIN experiment [5]. Moreover, ^{3}He to ^{12}C mass ratio could further clarify the inconsistency existing in the values of light masses from different world-leading experiments [2]. In this contribution, the present status of the experiment will be discussed.

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Photoemission Chronoscopy of the Iodoalkanes

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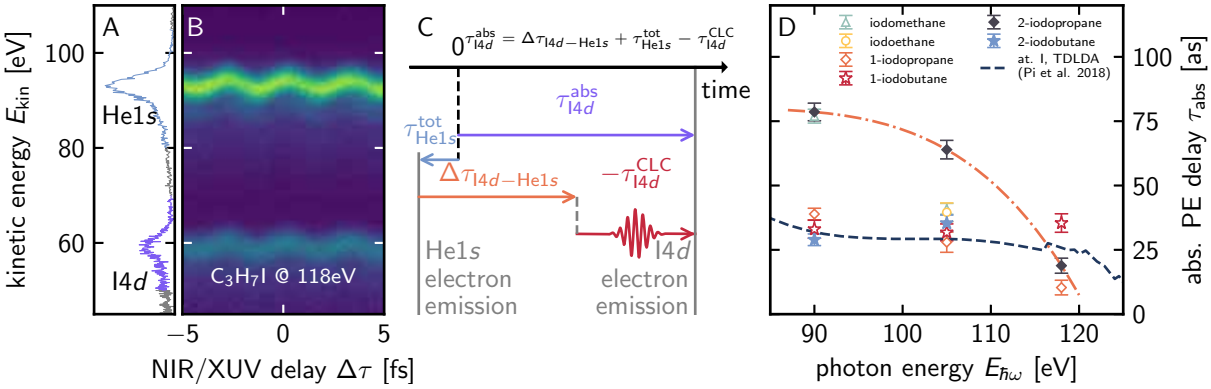

Recent theoretical simulations of several iodoalkanes, published in [1], suggest that the photoemission delay time increases with the size of the attached functional group. We find experimentally that this observation does not generalize to other iodoalkanes. Expanding the available data by studying primary iodoalkanes from iodomethane to 1-iodobutane and the secondary iodoalkanes 2-iodopropane and 2-iodobutane a surprising bifurcation of the excitation-energy dependence of the absolute photoemission times is found, that so far lacks explanation (panel **D**).

Photoemission timing of the I4*d* electrons for 90 eV, 105 eV and 118 eV is assessed via attosecond streaking (panels **A**, **B** and [4]) where the giant resonance in the I4$d \rightarrow \varepsilon f$ channel at 94 eV [6] serves as an intra-molecular time zero which we clock against the accurately known He1*s* [8] calculated with [11, 3, 2, 5]. Absolute photoemission times, isolated by subtracting the measurement induced Coulomb laser coupling delay [9] (panel **C**), are shown in panel **D** in comparison to a theoretical prediction τ_{at} for atomic Iodine [10]. No clear correlation between the size of the functional group and the observed deviation of $\tau_{\mathrm{I4}d}$ from τ_{at} is found where one might expect an increase. This is most evident for the case of 2-iodopropane versus 2-iodobutane at 90 eV and 105 eV (black diamonds vs. blue stars in **D**, red line was drawn as a guide to the eye) where the larger functional group exhibits a smaller delay. The currently available data on iodomethane furthermore suggests that even in the smallest iodoalkanes significant deviations from τ_{at} can occur, which has far-reaching implications for the use of Iodine for the purpose of absolute photoemission timing in condensed matter systems [7].

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Quantum technologies for single molecular ions

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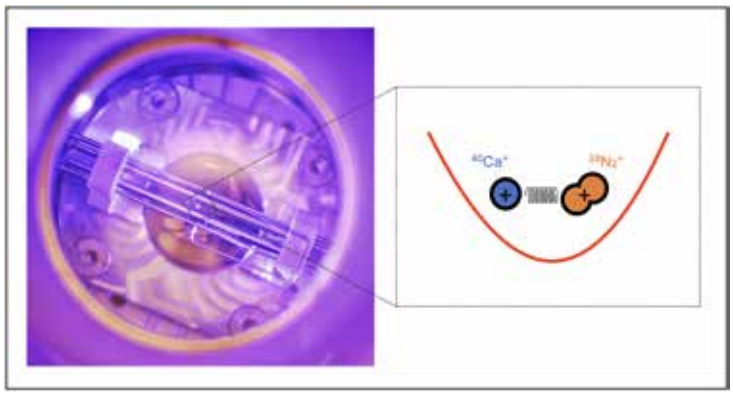

FIG. 1: Left: An ion trapping apparatus employed in order to confine single molecular ions for their precision investigations. Right: Illustration of a Ca^+–N_2^+ two-ion crystal trapped in the ion trap. The quantum states of the molecular ion can be probed and manipulated via the atomic ion by leveraging their mutual Coulombic interactions.

Over the past years, the development of experimental methods which enable the control of single isolated quantum systems has made impressive progress. While sophisticated techniques for the cooling and coherent manipulation of atomic systems are now well established, and form the basis for their application in modern quantum science including quantum computation, quantum simulation and precision measurements, their adaption to molecular systems has remained a persistent challenge. The complexity of the molecular energy-level structure poses, in general, severe difficulties for their translational cooling as well as the preparation, manipulation and non-destructive readout of individual molecular quantum states.

While the additional degrees of freedom offered by molecules impose challenges for their quantum control, they at the same time provide a rich playground for new applications. Molecules offer prospects as novel platforms for precise determinations of fundamental constants and their possible variations, for precision spectroscopic measurements, for tests of ab-initio calculations and molecular quantum theory, and for investigations of state- and energy-controlled atom-molecule and ultracold molecule-molecule collisions. Molecules are also being increasingly considered for development of new frequency standards and clocks.

Here, we present a complete theoretical and experimental toolbox for quantum control of single $^{28}N_2^+$ ions trapped in radio-frequency (RF) ion traps. In order to mitigate the aforementioned challenges, we employ quantum-logic protocols in which the quantum states of the molecular ion are controlled via a single co-trapped $^{40}Ca^+$ atomic ion. We present our techniques for the ro-vibronic state preparation and cooling of the molecular ion. We demonstrate a non-destructive quantum-non-demolition (QND) state-detection scheme for molecular-state readout with fidelities exceeding 99%. Additionally, we report our theoretical investigations of possible high-fidelity qubits and clock transitions in the spin, rotational, and vibrational degrees of freedom of N_2^+ spanning six order of magnitude in frequency. For highly precise and accurate spectroscopy of dipole-forbidden transitions of the molecular ion, we have setup a system of lasers traceable to the SI definition of the second via a phase-stabilized optical fiber network. The methods presented here lay the foundations for new approaches to precision investigation with molecules.

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Adatoms near graphene nanoantennas: interplay of optical coupling and electron tunneling

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Graphene constitutes an appealing platform for exploration of plasmonic phenomena, since it supports electrically tunable plasmons with relatively long lifetimes. For optical applications, finite nano-sized graphene flakes are of particular interest since they host plasmons with resonant frequencies in the visible range of the electromagnetic spectrum. The optical, plasmonic and transport properties of such nanoflakes can be notably modified by the presence of atoms adsorbed at the flake surface (*adatoms*). Here, we present a framework combining the master equation approach and the tight-binding approximation. It describes the electron dynamics in hybrid systems consisting of graphene nanoflakes with adatoms subject to external illumination [1,2]. The flake and the asatom can then interact through two distinct mechanisms, i.e. through electron tunneling or optically. We apply the presented model to investigate how emblematic quantum optical phenomena in two-level adatoms, i.e. coherent Rabi oscillations and incoherent damping, are modified in proximity of triangular graphene nanoflakes. Fig. 1 illustrates the Purcell effect modification by the exchange of electrons between the atom and the flake for an example set of parameters and for inverse quadratic scaling of the electron exchange rate with the atom-nanoantenna distance [2].

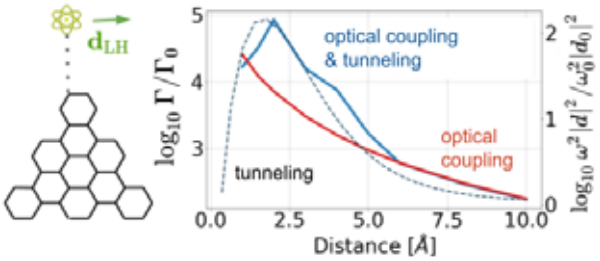

FIG. 1: Red solid line: Enhancement factor of the emission rate Γ of the adatom modelled as a dipolar emitter near a graphene nanoantenna due to their optical interaction, with respect to the free-space emission of a decoupled emitter Γ_0. As electron tunneling is included, the adatom and the nanoantenna hybridize. This leads to corrections of the transition dipole moment $\mathbf{d}_{\mathrm{HL}}$ and frequency ω_{HL} between the highest occupied (HOMO) and lowest unoccupied (LUMO) orbitals. Grey dashed line, y axis on the right: Resulting Weisskopf-Wigner spontaneous emission rate modulation. Blue solid line: Both effects combined. Quenching of the emission rate is found for small distances.

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Characterization of high-fidelity Raman qubits

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In quantum information and computation, very high fidelity of gate operations is required. Measuring tiny gate errors with high accuracy is a difficult task, which is traditionally done by randomized benchmarking. In this work we present a new method which allows to determine the gate errors of Raman qubits, in which the qubit states are coupled in a Raman transition via another state, thereby forming a three-state chainwise-connected system. The method is based on the repetition of the same gate sufficiently many times and thereby amplifying the tiny error to easily measurable sufficiently large values. In order to deduce the gate error from the amplified error, analytic connections between the single-gate and multi-gate propagators are derived for three-state Raman systems with two types of symmetries: Majorana and Morris-Shore. We extend these connections to arbitrary dimensions which paves the path toward tomography of qudits.

Disentangling Fundamental Processes of a Two-Level Wave Packet in Attosecond Transient Absorption Spectroscopy

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Attosecond transient absorption spectroscopy (ATAS) is used to study electron dynamics with the aim of unravelling ultra-fast phenomena in atoms and molecules. There have been many investigations on ATAS between bound states [**1**, **2**] , but few works has focused on the coupling of a prepared bound wave packet to both bound and continuum states [**3**]. A recent experimental investigation of the physical phenomena in this regime is presented in Ref. [**4**]. In order to disentangle the fundamental processes in this rich transient absorption regime, we have developed an analytical model which is able to account for the resonant (bound and continuum) and the off-resonant contribution. In the present work [**5**], we consider a hydrogen atom in an initial superposition state, comprised of two non-degenerate states, impinged upon by an attosecond pulse. We study the absorption depending on the relative wave packet phase of the prepared superposition. The analytical model, based on Coulomb functions, was compared with numerical simulations, conducted by solving the time-dependent Schrödinger equation, showing good agreement. The model allows us to explain that off-resonant contributions have a significant impact when lower energy states can be reached from the prepared wave packet, see for instance the transition to $1s$ from the prepared p wave packet in Fig. 1. The off-resonant contribution results in alternating absorption and emission structures over the relative wave packet phase, not present for the s wave packet. Thus, we have identified the mechanism causing emission structures from p wave packets. Using the model we have fully disentangled the complex ATAS spectra of two-level wave packets in atoms.

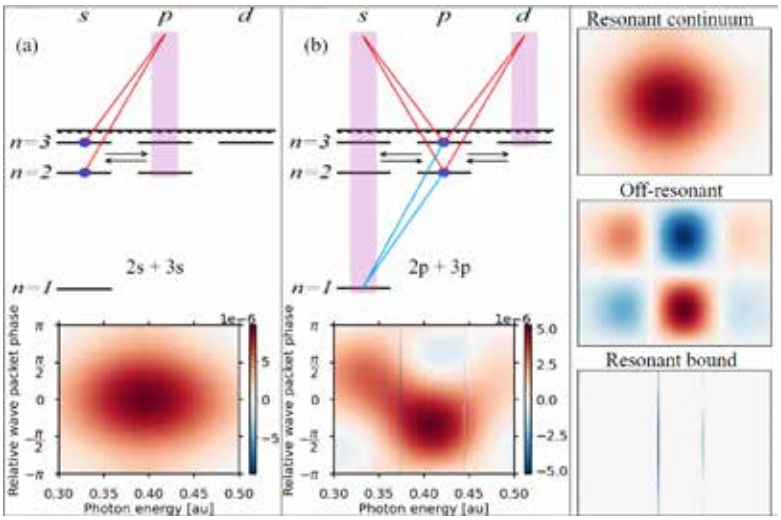

FIG. 1: (a) and (b) shows the schematic of the transitions handled by the model for the prepared superpositions 2s+3s and 2p+3p respectively, as well as the corresponding absorption profiles resolved over wave packet phase and photon energy. The rightmost figures show the contribution of the three absorption processes presented in the schematic, these are the resonant continuum (red lines), off-resonant (purple area) and resonant bound (blue lines) contributions.

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Schwinger Bosons for Density Matrices: Permutation Symmetry and Entanglement

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Quantum correlations are at the heart of quantum mechanics, a prominent example being the phenomenon of entanglement. This concept is well-understood for quantum systems consisting of distinguishable parties and found remarkable applications in quantum information (teleportation, algorithms, cryptography, etc). On the other hand, the entanglement of identical particles remains an open question [**1**, **2**], despite the exciting quantum properties they have to offer.

An important point to keep in mind is dissipation, inherent to any real-world quantum system. It points towards the density matrix formalism, which encompasses decoherence into the quantum description. Therefore, we aim to study the entanglement of indistinguishable particles on the level of density matrices.

We investigate this problem within a novel formalism, which resides on the idea of extending the traditional second quantization for state vectors:

$$|\psi\rangle \sim |i_1\rangle_1 \ |i_2\rangle_2 \ \ldots \ |i_N\rangle_N,$$

to the Liouville space of density matrices:

$$\widehat{\rho} \sim |i_1\rangle_1\langle j_1|_1 \ |i_2\rangle_2\langle j_2|_2 \ \ldots \ |i_N\rangle_N\langle j_N|_N.$$

We perform this extension and, as a result, get the occupation number representation and bosonic superoperators for density matrices. The bosonization is similar to the Jordan-Schwinger transformation [**3**], but formulated for density matrices describing open quantum systems. Our method takes advantage of the permutation symmetry and significantly reduces the number of relevant states. Crucially for our investigation, the algebra of bosonic superoperators is wider than spin algebra of $\widehat{\sigma}_{\mu,ij} = |i\rangle_\mu\langle j|_\mu$. It opens up new possibilities for analyzing density matrices, their properties and behaviour under the loss of particles and single-particle measurements, paving the way toward understanding the entanglement of indistinguishable particles.

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New Setup for High-Resolution Ion-Molecule Crossed Beam Imaging

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Detailed insight into the dynamics of elementary reactions in the gas phase can be obtained from crossed-beam reactive scattering experiments. With velocity map imaging (VMI), angle and energy differential cross-sections can be obtained [1,2]. In this contribution, we present the design plan and relevant simulations for an experimental setup to investigate ion-molecule reactions with higher precision than previously attainable. With our new setup, we plan to study fundamental astrophysically significant reactions such as $H_2^+ + H_2 \rightarrow H_3^+ + H$, with the aim to determine the product vibrational quantum states. H_2^+ ions will be created by laser induced ionization of H_2 with Nd:YAG laser so that they are mostly in the vibrational ground state [3]. In addition, according to our simulation, a proper shaping of the ionization volume and a very weak acceleration of the ions play a crucial role in deciding the ion beam energy resolution. The ion beam is overlapped with the beam of neutral molecules and the collision products are collected by the VMI spectrometer. We also plan a coincidence detection of both the ionic and neutral products after the reaction, which will be further implemented by a laser ionization scheme.

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Machine learning parameters of attosecond pulses based on photoelectron momentum distributions

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Complete determination of attosecond laser pulse parameters with a single atom target can be performed using an established CRAB method based on photoelectron spectroscopy [1], among other techniques [2]. In this work, we propose another, machine-learning-based algorithm of pulse characterization that utilizes photoelectron momentum distributions as an input. We train a Convolutional Neural Network, a standard choice for image processing tasks, on 6000 momentum distributions for various linearly polarized sin-squared pulses numerically simulated within the Strong Field Approximation (SFA) [3]. The data are labeled according to the pulse carrier frequency, carrier envelope phase, number of laser cycles and the target ponderomotive energy. We find that upon training the network can predict pulse parameters perfectly, see eg. FIG. 1. Our model may serve as a pretrained archictecture for further fine-tuning on real-world data from attosecond laboratory.

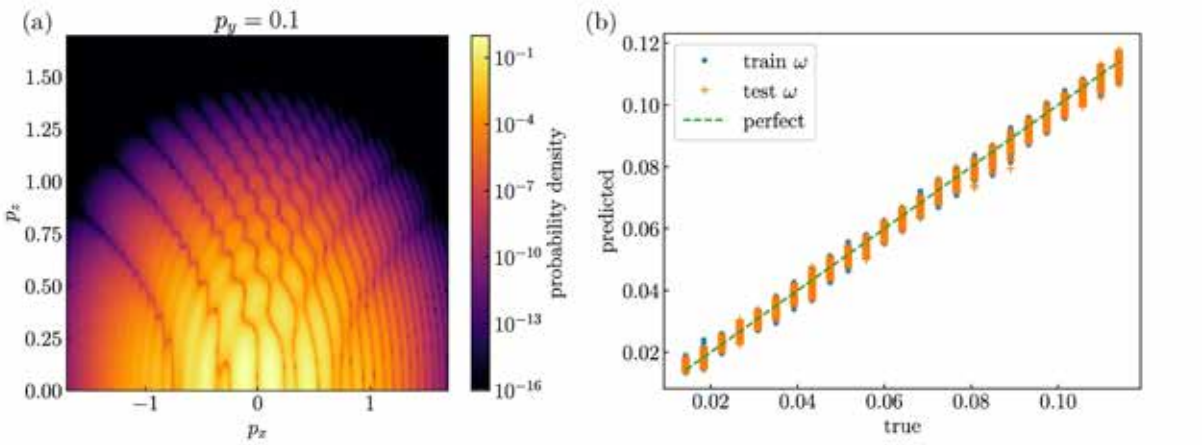

FIG. 1: (a) Photoelectron momentum distribution of Ar atom targeted by an attosecond pulse with carrier frequency 0.1425, carrier envelope phase $\pi/4$, 11 laser cycles and poneromotive energy 0.025 (all in natural atomic units), used as an input data. Training dataset corresponds to 6000 similar distributions. (b) Predicted carrier frequency as a function of true carrier. The network is evaluated on both training and test, i.e., unseen during training, data.

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The Nature of the Red Fluorescence States in the LHCII Protein Complex

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LHCII protein complex is one of many proteins embedded inside the thylakoid membrane of the chloroplast, yet it is greatly important for plant's survival mechanism. It is known to contribute to the processes of photosynthesis and non-photochemical fluorescence quenching (NPQ). The NPQ process involves charge-transfer states (CT) [1], which to this time have not been unambiguously located inside the LHCII.

One of the main signatures of the NPQ process is the red wing in the fluorescence spectrum of the LHCII aggregates and crystals [2]. To probe the origin of this signal, Chmeliov et. al. [3] performed the temporal and the spectral decomposition of the fluorescence spectrum of LHCII aggregates and trimers to find out that the nature of "red" emitting states is different from the quenching states. This claim was confirmed in the subsequent work [4], where the conditions were suggested for the "red" emitting state to also be responsible for non-photochemical fluorescence quenching. Recently Ostroumov et. al. [5] conducted a computational study of Chl oligomers to show that protonation of close lying amino acids in the LHCII can become the trigger for the quenching process. It was also concluded that the "red" emitting states are responsible for the process of NPQ.

The present computational investigation was conducted to find a consensus between the presented views. For this purpose, the Chl*a*610—Chl*a*612 dimer and the Chl*a*604—Chl*b*606 dimer were selected, because they both are formed from two close lying Chl monomers with high inter-pigment coupling [6]. The monomer geometries were first optimised at DFT/CAM-B3LYP/cc-pVDZ level of theory and structures were mapped according to the high spatial resolution LCHII protein crystal structure [7]. The same optimisation procedure was carried out for 11 neutral and positively charged amino acid (AA) structures, which protonation effects on the two dimers were investigated (1 AA for Chl*a*610—Chl*a*612 dimer and 10 AA's for Chl*a*604—Chl*b*606 dimer). It was assumed throughout the work, that the amino acids can only be protonated in their side chains. Finally, the excited state properties of assembled Chl—Chl dimers, Chl—Chl—AA (—AA^+) trimers and Chl—Chl—AA—AA (—AA—AA^+) structures were probed at the TDDFT/CAM-B3LYP/cc-pVDZ level of theory.

It was found that the protonation of most amino acids had a measurable impact on the CT state energies of both Chl dimers. However, the greatest effect was recognised due to the protonation of GLN131 amino acid close to the Chl*a*604—Chl*b*606 dimer – the process lowered the energy of the first CT state of the dimer by ~ 0.9 eV. The energy of the CT state was found to decrease even more upon the second protonation of the other few close lying amino acids.

The results suggest that the Chl*a*604—Chl*b*606—$GLN131^+$ trimer could correspond to the "red" emitting state in the fluorescence spectrum of LHCII aggregates. The possibility for the protonation of more than one amino acid explains the wide band visible in the fluorescence spectrum. Since the stroma of the thylakoid holds the proton excess and the Chl*a*604—Chl*b*606 dimer is close to the stromal side of the LHCII protein, this possibility is very likely.

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LOW-ENERGY ELECTRON IMPACT EFFECT ON THE AMINO ACID FRAGMENTATION: ISOLEUCINE CASE

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The theoretical study of the isoleucine fragmentation under low-energy electron impact was performed by using Becke's three-parameter hybrid functional approach, applying non-local correlation provided by Lee, Yang, and Parr (B3LYP) with the cc-pVTZ basis set implemented in a Gaussian package [1]. The structure of the conformers of the neutral and ionized isoleucine molecules was optimized without any symmetry constraints. The total energies of the conformers were compared to obtain the most stable ones. These structures were used for further investigation to obtain the ion structure of this amino acid as well as fragmentation products. The adiabatic ionization potentials were calculated to predict the fragmentation threshold energy. The appearance energy was calculated as the difference between the total energy of isoleucine and the sum of total energies of the fragments formed. Two conformers of the isoleucine molecules were found as the most stable ones (Fig. 1).

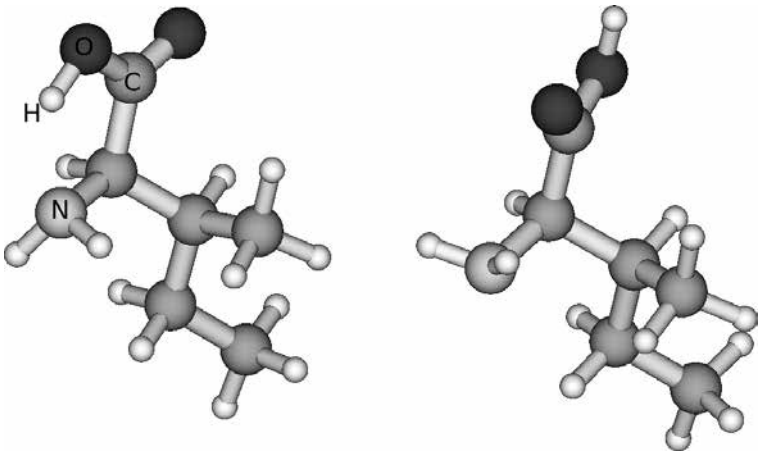

FIG. 1: The view of the most stable conformers obtained.

The results obtained coincide with our statements that the presence of the Van der Walls bond stabilizes amino acids [2]. The adiabatic ionization potential (IE) of 8.32 and 8.72 eV is obtained for each conformer under study. These IE values are similar to the appearance energies for the m/z=86 fragment (8.65 and 8.70 eV) produced from different isoleucine conformers. Hence, fragmentation of isoleucine could start along with its ionization. The reason for the m/z=86 fragment formation is losing COOH, i.e. fragmentation process common for various amino acids is realized in isoleucine, too. Comparison of the appearance energy of the CH_3N^+ and $C_2H_5^+$ (m/z=29) fragments allows us to predict the possibility of the H bonding reaction along with fragmentation. The chemical compositions and the paths of formation of the m/z=28, 30, 41, 57, 74, 75 fragments are also obtained based on the theoretical results.

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Acknowledgments

This work was carried out within the CA18212 – Molecular Dynamics in the GAS program. The authors are grateful for the high-performance computing resources provided by the Information Technology Open Access Centre of Vilnius University.

Tunable Optical Parametric Amplification of Subnanosecond Light Pulses in LBO and BBO Nonlinear Crystals

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Optical parametric generators and amplifiers are the widely utilized tools for generation of the widely-tunable laser pulses. The femtosecond and nanosecond pulses are available and utilized in various practical as well as scientific applications. However, the parametric generation of subnanosecond pulses (0.1–1 ns) is still a challenge due to the laser induced damage the threshold of which is close to the optical parametric generation threshold.

In this work, we present the results of our recent study on the optical parametric amplification of the subnanosecond pulses in the nonlinear lithium triborate (LBO) as well as beta barium borate (BBO) crystals. The two experimental schemes were similar, but with a different nonlinear crystal. The advantage of LBO crystal was the small walk-off angle between the pump and generated waves [1], while the BBO crystal provided larger nonlinear coupling. In this study, we put more accent on the theoretical simulations that supplement the experimental investigation.

In the experiment, the pump of 355 nm wavelength and pulse duration of 500 ps was implemented. As the idler wave (seed), the supercontinuum at 1064 nm peak wavelength was used. The supercontinuum radiation was generated by pumping the photonic crystal fiber with the subnanoseond pulse at 1064 wavelength. The output radiation was a subnanosecond pulse with a wide spectrum range. Such seed allowed the generation of the widely-tunable visible signal pulses. The numerical simulation of the parametric amplification was performed with the use of the experimentally recorded seed spectrum. Three wave interaction equations including dispersion terms were simulated by the use of the split step Fourier transform method [2]. The resulting signal spectra are presented in Fig. 1. As we can see, the signal wavelengths cover the range from 460 nm to 710 nm what is in good agreement with the experimental data. The maximum signal output is at 532 nm wavelength that corresponds to the seed peak at 1064 nm. Besides the spectra calculations, the temporal and power characterization was also performed.

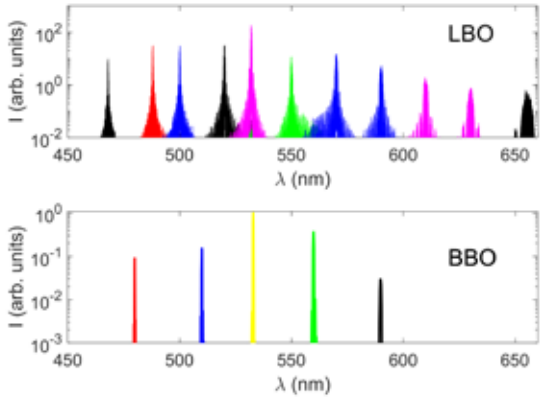

FIG. 1: Numerically simulated signal spectra in LBO and BBO crystals.

This work has received funding from European Regional Development Fund (project No. 01.2.2-LMT-K-718-03-0004) under grant agreement with the Research Council of Lithuania (LMTLT).

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Interferometer with Bose-Einstein Condensate based on quasi-Bragg diffraction

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Applications of atom interferometers exist in various fields. They are used for inertial sensors, geophysics, fundamental constant measurements or fundamental physics tests. Here, we present an atom interferometer with a truly macroscopic spatial separation between the interferometer's arms. This specificity allows to shape electromagnetic and gravitational potentials. This approach paves the way for new measurements using geometrical phases in fundamental physics and metrology.

Our interferometer uses the quasi-Bragg diffraction of a Bose-Einstein condensate. I will present a characterization of an atom Mach-Zehnder interferometer based on quasi-Bragg diffraction up to fifth diffraction order. We demonstrate [1] that non-adiabatic losses impact diffraction phase shifts and create parasitic interferometer paths which can bias the phase estimation.

I will also show a Large Momentum Transfer interferometer based on sequential quasi-Bragg diffraction. We achieved up to $104\hbar k$ momentum separation between the two arms with a visibility of 19% and keeping the phase sensitivity.

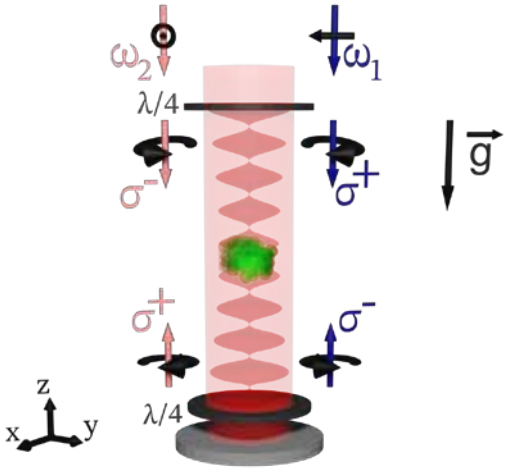

FIG. 1: Ultracold-atom on an vertical optical lattice, in retro-reflected configuration, created by two laser beams at frequencies ω_1 and ω_2 with orthogonal polarizations.

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Complexity of the photoelectron holographic structures induced by strong field laser pulses in atomic targets

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Nowadays, the laser-induced electron diffraction (LIED) imaging technique uses the self-imaging of the molecular target by its own re-scattered electrons liberated by strong-field interaction to image the nuclei motion in molecules [1, 2]. Those electrons must be sufficiently energetic to induce a possible structure retrieval from the diffraction pattern. On the other hand, the re-scattered electrons are also the backbone of the strong-filed attosecond photoelectron holography (SFAPH) imaging technique because they represent the probe electron beam of the target structure. This latter is based on the interference scenarios between the scattered and unscattered electrons liberated in the same optical cycle. Along this line an intensive work has been devoted to understand the sub-cycle electron dynamics from the momentum distributions of photoelectrons (holograms) [3, 4]. The principle of photoelectron holography is based on the presence of two coherent electron wave packets (the re-scattered and direct electron wave packets) which interfere between each other due to their phase difference forming holographic structures in the PMD. We found that the formation of the most known holographic structures strongly depend on the number of optical cycles (see Fig. 1.). In particular for the case of the three-cycle pulse, the PMD shows an interesting features, i.e. one can see the coexistence the fishbone-like, shield like and fanlike holographic structures in the same holographic pattern (see Fig. 1c). Thus, the three-cycle pulse could be a good pulse candidate to investigate the holographic structures. In addition, we can also note that the ATI rings are less pronounced and will not wash out the holographic patterns unlike the multi-cycle pulses (see Fig. 1d). The effects of the intensity and wavelength of the laser pulse to the PMD show that they are responsible for the interference fringes density in the holographic structures. We found in particular, that the fan-like structure is very sensitive to the wavelength variation. It is interesting to note that this fan-like structure can disappear by applying longer wavelengths [5].

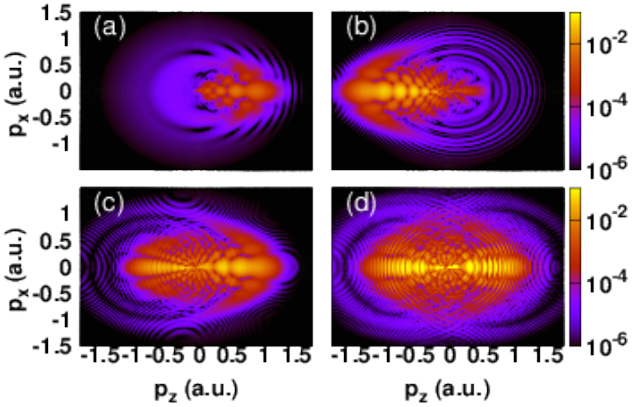

FIG. 1: PMDs corresponding to the ionisation of hydrogen atom induced by a strong laser pulse of a carrier wavelength of 800nm . The panels correspond to different number of optical cycles N of the pulse. (a): N=1; (b): N=2; (c): N=3 ; (d): N=8. The laser intensity and the carrier envelope phase are fixed at 1×10^{14} W/cm^2 and 0 degree respectively.

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Role of Symmetry in Environment-Sensing Mechanism of BODIPY-Based Molecular Dyes

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A widely-studied range of molecular sensors for measuring viscosity (and possibly temperature and polarity as well [1]) in microscopic environments are based on BODIPY (boron-dipyrromethene) molecule with a rotation-capable chemical group attached. The viscosity-sensitivity mainly depends on the presence and height of the moderate (50–200 meV) energy barrier between the fluorescent state of the optically-excited molecule and a non-radiative decay channel; this mechanism can be modeled, as a first approximation, by the evolution of the electronic excitation along the potential-energy curve of the lowest excited state with respect to the rotation angle [2]. However, non-trivial structure of base and rotation groups presents several challenges for such an approximation. First, a single dihedral (4-atom) angle was found to be insufficient to properly define the angle between BODIPY and rotator, both in cases where rotation group itself is asymmetric (Fig. 1A) and in cases where intrinsic symmetry is preserved but not apparent in realistic conditions, such as after the observed bending of the base in BODIPY-phenyl [2] (Fig. 1B). Second, use of asymmetric rotation groups does not result in a forced extremum at the 0° rotation angle that simplifies the model for many popular BODIPY-based sensors, such as functionally-symmetrical BODIPY-C_{10}.

The presented study, aided by quantum chemical computations based on density-functional theory, explores the potential energy surface of the lowest excited electronic state in several chemically-related BODIPY compounds. A reaction coordinate based on the average of opposite dihedral angles is shown to better estimate the actual rotation than a single dihedral. The changes in the shape of the energy surface and the emergence of the barrier upon symmetrization of a hydrocarbon-based rotation group are also investigated in more detail.

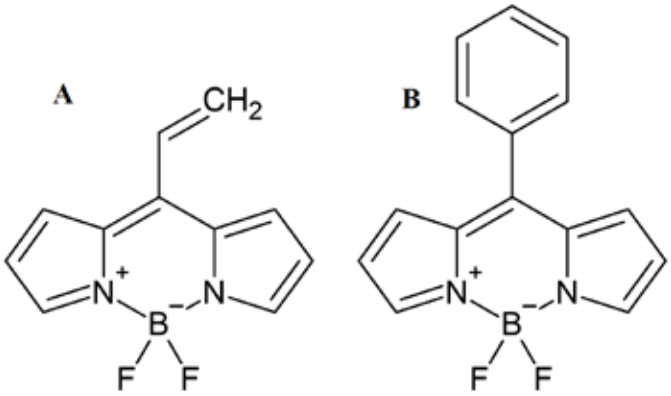

FIG. 1. Molecular structure of BODIPY compounds with asymmetric vinyl group (A) and C_{2v}-symmetric phenyl group (B)

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Collisional losses of ultracold molecules due to intermediate complex formation

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Understanding the sources of losses and chemical reactions of ultracold alkali-metal molecules is among the critical elements needed for their application in precision measurements and quantum technologies. Recent experiments with nonreactive systems have reported unexpectedly large loss rates, posing a challenge for theoretical explanation [1-3]. Here, we examine the dynamics of intermediate four-atom complexes formed in bimolecular collisions [4]. We calculate the nuclear spin–rotation, spin–spin, and quadrupole coupling constants for bialkali four-atom complexes using *ab intio* quantum-chemical methods. We show that the nuclear spin–spin and quadrupole couplings are strong enough to couple different rotational manifolds to increase the density of states and lifetimes of the collision complexes, which is consistent with experimental results. We also reveal that the interaction-induced variation of electron spin–nuclear spin couplings explains the recently observed long lifetime of alkali-metal three-atom complexes formed in atom-molecule collisions [5]. Finall, we propose further experiments to confirm our predictions.

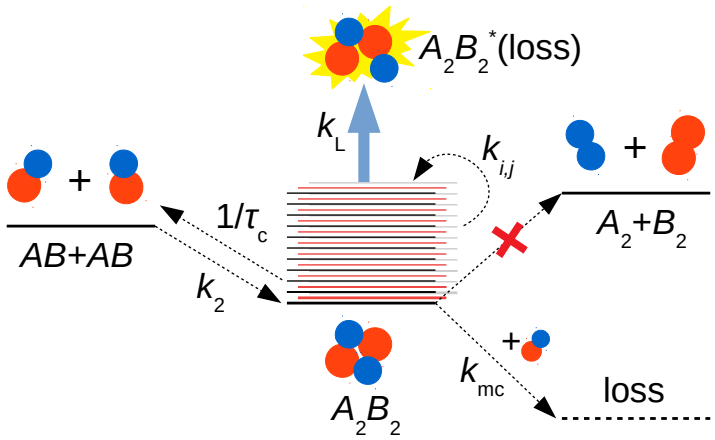

Figure 1: Schematic representation of the competing processes in ultracold nonreactive bimolecular $AB+AB$ collisions. Four-atom A_2B_2 complexes form with the rate constant k_2 and spontaneously dissolve with the rate constant $1/\tau_c$. They change their internal spin states with the rate constants k_{ij} and can be lost due to the laser photoexcitation with the rate constant k_L and collisions with other molecules with the rate constant k_{mc}. In this work, we consider systems where a direct chemical reaction to $A_2 + B_2$ is energetically forbidden.

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High robustness quantum walk search algorithm with qudit Householder traversing coin

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Quantum random walk search is quantum algorithm for search in unordered database with arbitrary topology [1]. The walk-coin is an operator that determines the probabilities to go in each direction. There are different ways to construct the walk-coin, for example in [2] it is built by a generalized Householder reflection. Some topologies as the hypercube have important practical use [3].

In [4] a quantum random walk search on hypercube, with walk-coin constructed by generalized Householder reflection and additional phase, has been studied. We have shown that this modification of quantum walk search algorithm is much more robust against deviations in the walk-coin parameters if an appropriate relation between them is maintained. Functions giving the most stable constructions of the quantum algorithm for different sizes of the coin were found.

Here we present an extension to our previous work by using a coin constructed by qudits. We investigate in more detail the robustness of quantum random walk search as a function of the coin register size [5]. We find optimal values for the walk-coin parameters in our modification of the quantum walk search giving more stable implementation of that algorithm. Examples for number of cases are presented as an illustration.

This work was supported by the Bulgarian Science Fund under contract KP-06-M48/2 /26.11.2020.

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Non-thermal desorption from molecular ices: quantifying the role of Auger electrons in XESD

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X-Ray irradiation of interstellar ices analogues has been shown to produce non-thermal desorption of intact molecules and their fragments (e.g. H_2O [1] and CH_3OH [2]), as well as contributing to the chemical enrichment of the gas phase [2,3]. The proposed desorption mechanism is X-ray induced electron stimulated desorption (XESD), which involves the Auger decay of the excited/ionised molecules following X-ray photon absorption [1,2]. The subsequent thermalization of the Auger electron in the ice, and the cascade of secondary low energy electrons it creates, would be responsible for most of the observed desorption and chemistry [4].

With the aim of quantifying the role of the released electrons in the desorption process and of comparing it to the global X-ray desorption yields, we have irradiated pure methanol ices deposited at 23 K with 505 eV electrons under UHV conditions, to simulate the Auger electron originating from a O 1s core absorption in the ice. The effects of irradiation flux and ice thickness on desorption were studied in the range of $0.8 – 7.0\times10^{13}$ $s^{-1}cm^{-2}$ and in the multilayer regime, respectively. Desorption of neutral fragments was probed with a Quadrupole Mass Spectrometer (QMS) during irradiation. After calibrating the QMS signal using Temperature Programmed Desorption experiments (TPD) we derived desorption yields in molecules per incident electron.

Desorption of the parent molecule (CH_3OH) was observed and the corresponding yield, 0.15 molecule per electron, is consistent in order of magnitude with the yield derived in X-Ray irradiation experiments [2]. Electron irradiation was observed to lead to the synthesis and desorption of stable products. In decreasing desorption yield (molecules per electron): CO (1.1), CO_2 (0.25), CH_4/O (10^{-1}), H_2O (0.07), H_2CO (0.04) and C_2H_6 (0.03). Other less abundant but heavier products were also observed, as evidenced by m/z 46, 60 and 61. Qualitative data from post-irradiation TPD corroborates the presence of irradiation products and supports the interpretation of the mass spectra recorded during electron irradiation.

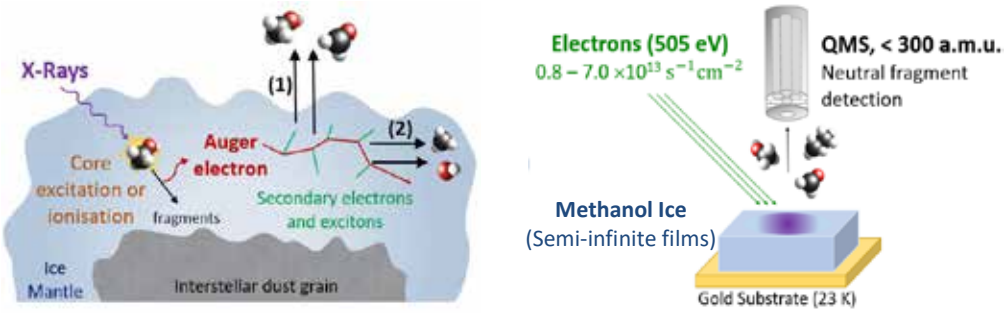

Figure 1: (Left) Simplified diagram of the thermalization path of an Auger electron in the ice mantle of an interstellar grain, which can lead to (1) desorption and (2) fragmentation. Reactive fragments created in the ice can react to form new products, which can subsequently desorb. (Right) Scheme of the electron irradiation experiments done.

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Towards Crossed-Beam Ion-Molecule Coincidence Imaging

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Crossed-beam Velocity Map Imaging (VMI) has provided a detailed insight into the reaction mechanisms of many ion-molecule reactions [1–3]. The obtained angle- and energy-differential cross-sections show the dynamics of the scattering processes by measuring the velocity distribution of ionic products with a VMI-spectrometer. Due to the nature of the detector system, we have not been able to measure neutral products by this means in past experiments. In this contribution, we present the currently constructed setup for the ionisation of the neutral hydrogen product in reactions such as $O^- + H_2 \rightarrow OH^- + H$ or $H_2^+ + Ne \rightarrow NeH^+ + H$. This ionisation will enable us to detect the ionic product as well as the now-ionised H-atom in coincidence, which will give us access to a kinematically complete picture of the scattering processes, as well as drastically improve the energy resolution of our newly developed VMI spectrometer. This will allow us to resolve the molecular vibrational levels of the products in these reactions. The unprecedented energy resolution that will be achieved with this experimental setup will give us the opportunity to study the possible existence of quantum scattering resonances in those reactions. For the reaction involving Ne and H_2^+, we plan to provide benchmark data for the quantum reactive scattering in three-atom collisions and explore the reaction dynamics predicted by [4]. The status of the construction of the setup and the implementation of the laser setup will be presented.

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Algebraic Methods for Precise Atomic Structure Calculations

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Atomic physics is still at the frontier of our exploration of fundamental physical laws [1]. The comparison of the theoretical and experimental values of the parity non-conservation (PNC) amplitude constitutes one of the most stringent tests of the Standard Model. However, at the present, there are several calculations on the cesium atom that differ at a sub-percentage level [1], [2]. In view of the importance of accurate PNC amplitude calculation, we have decided to perform independent calculation. We propose the use of Sturmian basis set, instead of the B-spline basis set used in previous calculations [3], [4], for relativistic atomic structure calculations and we describe numerically stable algebraic calculation of one- and two-particle radial integrals. The method is illustrated on the basis set independent calculation of energies, electric dipole moments, hyperfine integrals and parity non-conserving amplitude for Cs in the Dirac-Hartree-Fock approximation with frozen core orbitals. Some of the previously reported results are found to be strongly basis dependent.

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Analysis of variable stars in binary systems from TESS observations

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Binary stars are crucial for understanding the evolution of stars and their influence on the formation of clusters, galaxies and their structure.Furthermore binary systems with variable component represents significant enough fraction of binary stars systems and they are ideal objects for determine stellar evolution and properties of the stars.

The brightness of eclipsing binary system changes due to the relative movement of two stars. From the observers perspective, as they move, the stars obscure each others light, leading to significant brightness changes. Photometric and spectrometric observations of eclipsing binary stars and analyses of them allow us to more accurately determine the parameters of the stars. Studies of binary stars provide an opportunity to find out not only the parameters such as luminosity, size and temperature, but also masses of the components. While determining individual star mass is a difficult task and could be done from color–magnitude diagrams or mass–luminosity relation, but analysis of gravitational interaction of stars in binary or multiple systems with each other makes this task easier.

Variable stars are still relevant to this day, because different oscillation modes of a variable star are sensitive to different layers of the star and contain information about the internal structure of the star. Variable stars can be found over the entire HR diagram and new variable stars are still being discovered to this day.

Variable stars are studied by a branch of astronomy called asteroseismology that aims to understand the structure and evolution of stars by examining their oscillations[**1**]. Asteroseismology became more popular, as many space telescopes were launched,that can produce continuous and more detailed lightcurves than ground based telescopes.

In 2018, a TESS (Transiting Exoplanet Survey Satellite)[**2**] space telescope was launched. TESS originally was designed to search for exoplanets, but it is a perfect tool for observations of variable and eclipsing binary stars too. Therefore, we decided to analyse all known Algol type eclipsing binary stars observed with TESS and create a catalogue of eclipsing binary stars that contain variable stars. We obtained a list of known eclipsing binary stars from AAVSO International Variable Star Index VSX catalogue[**3**]. Among known 95893 Algol binary systems, we found that 13045 are binary stars with periods longer than 4 days. 10318 of them were observed with TESS. We downloaded their light curves observed with 2 min and 30 min cadences. Using binary stars modeling tool Phoebe[**4**], we removed eclipses and analysed remaining light curves for stellar variability. We found more than 500 binary stars with variable component.

Binary stars usually share similar evolution history and by combining results from asteroseismic analysis of a variable component with results obtained from observations of eclipses, we can more accurately determine parameters of stars in binary system, their evolution and internal structure.

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Formation of anion C_2H^- in reaction of O^- with C_2H_2 studied with 22-pole RF ion trap at temperatures 40 K - 300 K

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Anions, negative ions, play an important role in many gaseous environments, from planetary atmospheres to interstellar clouds. First detection of an anion in space was in 2006 with many other observations of anions following after [1, 2]. Anions also play an important role in numerous plasma technology applications and ion sources.

In present study, we investigate the first step of formation of linear carbon chains. These molecules are not common on Earth and a mechanism of their formation is not yet fully explained. Several studies were recently performed with one example being [3]. Formation of negative carbon chains is coupled with a formation of neutral molecules and a carbon chain growth for a creation of more complex molecules. Anion C_2H^- is a possible first step in formation of complex carbon chains. It has not been detected yet in interstellar space, even though its neutral C_2H is a well known and abundant molecule in space. Chemical models predict greater stability for more complex carbon chains than for its simpler variants. According to [4], there are multiple reactions leading to creation of C_2H^-. We focus on a reaction of oxygen anion O^- with acetylene C_2H_2.

The reaction is being studied using a 22-pole RF cryogenic ion trap apparatus [5] at low temperatures. The trap consists of 22 rods using radio-frequency field for radial confinement and two electrostatic potentials on the ends of the trap for axial confinement. The apparatus is build using UHV technology. During measurements, typical number densities of reacting molecules are $\approx 10^7 - 10^9\,\mathrm{cm}^{-3}$. Two stage coldhead, which is a closed cycle helium refrigerator, is responsible for cooling the trap from room temperature down to tens of kelvin. Ions are created by electron impact from N_2O gas in an ion source. Ions are extracted from the ion source and subsequently filtered by a quadrupole mass filter. Afterwards, oxygen anions are caught in the trap. Mixture of acetylene and helium is injected directly into the trap. After a well defined time, trap is opened and ions are analyzed by the second quadrupole, which is used as a mass spectrometer. Finally, we detect individual ions by microchannel plate detector. Following reaction branches were expected:

$$\begin{aligned} O^- + C_2H_2 &\rightarrow C_2H_2O + e && \approx 94\%;\ \Delta H_0 = -3.9\,\mathrm{eV} \\ &\rightarrow C_2H^- + OH && \approx 5\%;\ \Delta H_0 = -1.1\,\mathrm{eV} \\ &\rightarrow HC_2O^- + H && < 1‰;\ \text{exothermic} \\ &\rightarrow C_2^- + H_2O && < 1‰;\ \Delta H_0 = -0.5\,\mathrm{eV} \end{aligned}$$

Presented results show the reaction of O^- with C_2H_2 having a small temperature dependence for the overall reaction rate coefficient from 300 K down to 140 K. Value of the reaction rate coefficient is approximately $1 \cdot 10^{-9}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$, which is close to Langevin's rate constant $1.4 \cdot 10^{-9}\,\mathrm{cm}^3\,\mathrm{s}^{-1}$. Ratio of C_2H^- formation in respect to electron detachment shows very small dependence on temperature as well. This work was supported by the Czech Science Foundation 20-22000S and Charles University Grant Agency 376721. Further studies of C_2H^- formation are being prepared for realization.

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Photoabsorption spectra of CsI plasmas in the 18-25 eV photon energy region.

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We report photoabsorption measurements on CsI plasmas in the 18-25 eV photon energy region using a dual laser plasma technique. Specifically, one plasma acts as a sample and the other as a vacuum ultraviolet (VUV) continuum light source. Laser produced plasmas (LPPs) have played a profound role in the ever-growing repertoire of the innovations associated with the fields of pulsed laser deposition (PLD) [1] and Extreme-UV lithography (EUVL) [2]. Spectroscopically, LPPs have attracted significant attention due to the simultaneous presence of atoms, molecules and ions in a range of different quantum states (e.g., low-lying excited states [3] and/or metastable states [4]). However, the inherently rich composition of LPPs renders the corresponding spectroscopic investigations challenging.

In this work, features associated with Cs atoms and Cs^+ ions were observed by varying the interlaser time delay. As shown in Fig.1, obtained at an inter-laser delay of 350 ns, the resulting spectrum is dominated by Cs^+ ions and is compared with previously reported measurements [5]. In addition, the $5p^6$ $(^1S)^1S_0$ -$5p^5 10d^1(^2P)^3P_1$ transition has been observed, for the first time to our knowledge. At longer time delays, spectral signatures associated with transitions from the $4d^{10}5s^25p^67s^1$ low-lying excited state in atomic Cs are identified with the aid of Hartree Fock with Configuration Interaction (HFCI) calculations.

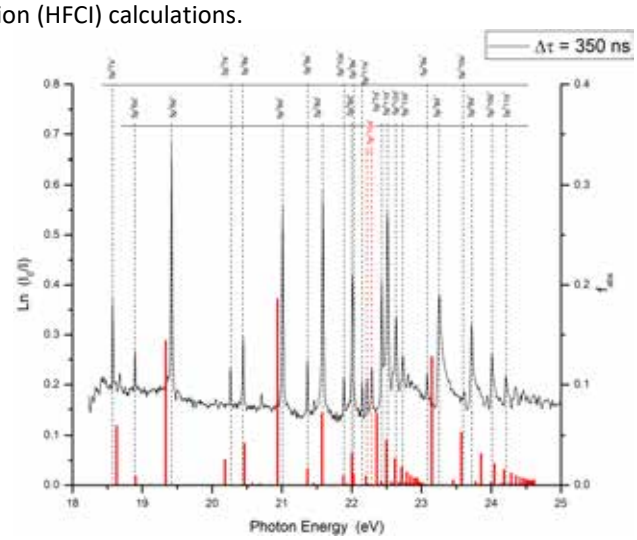

FIG. 1: The experimental photoabsorption spectrum of a Cs plasma for an inter-laser time delay of 350 ns (black solid line). Also shown are the calculated fabs values for different Rydberg series in Cs^+ (red sticks).

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The Role of the Operating Position of Mercury Capillary Light Sources

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For the determination of pollution, including heavy metals like mercury in the environment, the atomic absorption method is often used [1]. To reach low levels of detection in metal analysers, an optically thin light source with narrow and intense spectral lines is necessary [2].

In the present paper, the role of the operating position of low-pressure mercury capillary electrodeless light sources is studied (see Figure 1) which are important for the practical application of the capillary sources in portable spectroscopic mercury analysers. Due to the small dimensions and plasma-wall interaction, experimental investigations of capillary plasmas is extremely difficult. In this work, a combination of optical spectral measurements and the emission tomography method is used to investigate the spectral properties of a 2 cm long Hg capillary with the buffer gas Ar and Xe, the reservoir diameter is about 1 cm, in three working positions – horizontal, vertical with Hg reservoir up and down. The CRi Nuance EX camera with a liquid crystal tuneable filter, which allowed spectral scanning with 1 nm steps in the spectral region from 450 nm till 950 nm was used. The capillary lamp was operated by the HF generator of 4 V voltage and 300 MHz frequency.

The authors found that the reconstructed profiles for different Hg/Ar capillary lamp positions of the mercury spectral line of 546.07 nm have different shapes. This effect can be associated with the phenomenon of radial cataphoresis. The position of the reservoir (up or down) in the vertical orientation of the capillary tube affects the brightness of the radiation in the mercury spectral lines. However, this practically does not affect the radial profile of spectral lines. The same capillary lamp position in all measurements should be recommended.

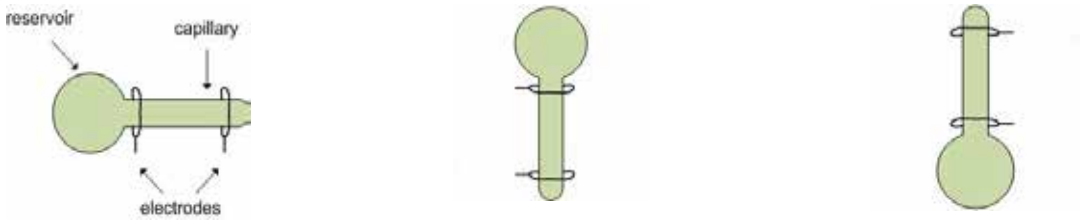

FIG. 1: Three capillary lamp positions studied in this work: the reservoir is oriented relative to the capillary tube a) laterally, b) upwards, c) downwards. Ring electrodes are schematically shown.

The research was supported by the Latvia Council of Science Project No. lzp-2020/1-0005.

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A Transition Metal to Ligand Bonding Nature: How a Quantum Chemical Study of Ru η3-allyloxapyridyl Complex Reveals the Operation of the Dewar–Chatt–Duncanson Model

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Understanding of a transition metal to ligand bonding nature is important for characterization of experimental observations. One of the methods to explain these interactions is the Dewar–Chatt–Duncanson (DCD) model application. However, in most applications (for example explanation trends in vibrational spectroscopy, chemical properties of molecules) the validity of the DCD model is based only on an assumption. In this work the new intermediate Ru η3-allyloxapyridyl complex has been studied aiming to illuminate DCD [electron donation/back-donation (D/BD)] model operation by quantum chemical calculations. A non-standard, alternative calculation scheme integrating the density functional theory along with the natural bond orbital (NBO) analysis and map of electrostatic potential has provided new insights into the electronic structure of the complex presenting it in a Lewis structure. The electron donating, accepting contribution of Ru to ligand bonding in BD has been estimated by Weinhold's perturbation theory. This allowed quantifying D and BD contribution to the stabilization of the complex Lewis structure by deletion of selected Fock-matrix elements from the basis set. The Lewis energy gets lowered mainly by BD contribution from Ru d NBOs into the C2 atom of allyl ligand. Finally, the outcomes of calculations reveal: that Ru to ligands is bonded in donor-acceptor fashion; the complex embodies nucleophilic character accumulated on the lone pairs of oxygen atom in oxabenzyl group. The nucleophilic sides suggested by calculations supports the reactivity trends of the complex in the catalytic reaction cycle. Calculated properties correlate well with experimental observations.

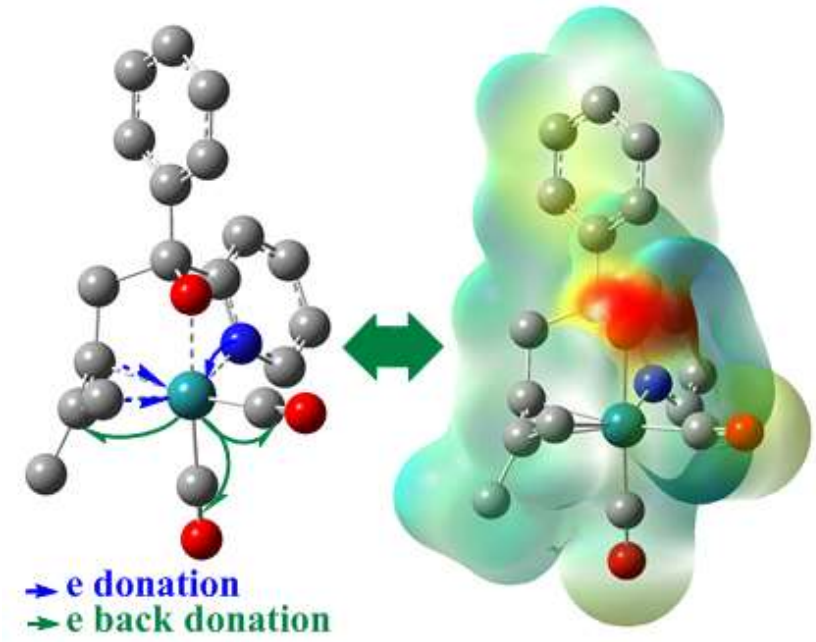

FIG. 1: The Lewis structure and the Map of electrostatic potential calculated for the Ru η3-allyloxapyridyl complex.

Computations were performed on resources at the supercomputer "VU HPC" of Vilnius University in Faculty of Physics location.

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Redox properties of 2-arylamino-1,4-benzoquinones. Theoretical study of redox potential

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1,4-Benzoquinone (BQ) and its variously modified derivatives (Q) are often used in bioelectrochemistry [1] as a mediators in bioelectrochemical analyzers. Depending on a medium, the mediator can undergo a variety of reduction-oxidation processes, from a simple one- or two-electron transfer to the combined two-electron and two-proton processes converting quinone (BQ or Q) molecules to hydroquinone (H_2BQ or H_2Q) and vice versa [2]. In this way, the mediator exchanges electrons with the electrode and the enzyme and protons with the solvent.

In this work, the oxidation-reduction properties of BQ and H_2BQ as well as their 2-arylamine-substituted derivatives Q and H_2Q by donation or acception of two electrons and two protons were investigated in order to determine how Q and H_2Q substituents affect redox properties compared to unchanged BQ and H_2BQ. The molecules studied are shown in FIG. 1.

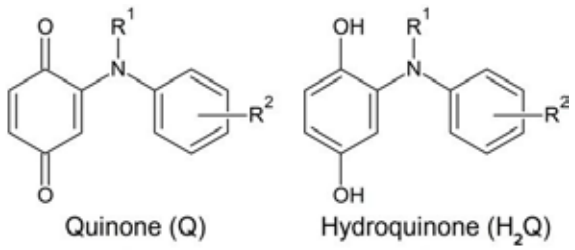

FIG. 1: Structures of Q and H_2Q under investigation

Q	R^1	R^2
1	H	3-NO_2
2	CH_3	H
2a	CH_3	H
3	H	2-OCH_3
4	H	4-OCH_3
5	H	2-F
6	H	4-F
BQ	–	–

The experimental trend of the standard electrode potential on the pH equal to –60 mV/pH [3] clearly indicates participation of two electrons and two protons in redox process. This is a well-known fact [2] that quinones in acidic environment undergoes such reduction-oxidation reaction in one step. To calculate the standard electrode potential in relation to the standard hydrogen electrode (SHE) we have to calculate the Gibbs energies G of the two half-reactions [4]. One of them is the reduction of Q to H_2Q by addition of two electrons and two protons. Another is the process going at the SHE. To simplify calculations, we combined these two half-reactions as one reaction

$$Q + H_2 = H_2Q$$

Standard electrode redox potential E^0 vs SHE is related with the Gibbs energy change ΔG for the above presented reaction

$$- nFE^0 = \Delta G$$

where n = 2 is the number of electrons participating in the reaction and F is Faraday constant. Calculation of Gibbs energy change at the standard conditions is straightforward and can be expressed as follows

$$\Delta G = G(H_2Q) - G(Q) - G(H_2)$$

Calculations were performed using the Gaussian 09 program for molecules in gas phase and in water solution at B3LYP/6-311 + g(d,p) level of theory. The calculation results agree well with the experimental data [3].

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Generalization of the Post-Collision Interaction Effect: From Gas-phase to Solid-state Systems as Demonstrated in Thiophene and Thiophene-based Conjugated Polymers

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After high-energy photons ionize the atomic core shell close to the ionization potential (IP), a slow photoelectron leaves the atom, interacting with the ionic field. Decay may take place via emission of an Auger electron (AE), which may interact with the photoelectron (PE). The Coulomb interaction between the three parties is known as post-collision interaction (PCI). The energy exchange arising from PCI between the ejected AE, PE and the remaining ion, visibly affects electron spectra in two ways: the energy distribution represented by the lineshape becomes distorted, and the position of the lines in the energy spectrum may shift substantially [1]. Thus, understanding the PCI mechanism and its manifestation in solids is of significant practical interest. Techniques such as X-ray photoelectron spectroscopy and Auger electron spectroscopy are widely used in material science for surface analysis of a vast range of materials. The accuracy of these methods strongly relies on diligent description and interpretation of the shape and energy position of spectral lines, which can be considerably affected by PCI. The PCI phenomenon has been extensively studied in gaseous systems [2, 3]. However, little is known on the manifestation of PCI in solid-state systems.

Using the HAXPES end-station at the GALAXIES beamline of the SOLEIL French synchrotron facility [4], we measured high-resolution KLL Auger spectra at photon energies between 0 and 200 eV above the sulfur 1s IP of: 1) gaseous thiophene, a heterocyclic aromatic molecule, 2) polythiophene (PT), a thiophene-based **π**-conjugated polymer, in powder form, and 3) P3HT, another thiophenic polymer, as a thin-film.

A visibly stronger PCI shift was observed in PT and P3HT compared to thiophene. Theoretical calculations attribute these observations to two main factors: **1)** electron scattering contributions, where the PE can lose kinetic energy through inelastic scattering processes, while elastic scattering reduces the photoelectron path within the solid by the time Auger decay takes place, leading to an increase of PCI. **2)** the dielectric medium screens electronic charges affecting the Coulomb interaction between PE and AE, leading to a reduction of PCI. Ultimately, however, electron scattering contributions overtake whatever diminishing effects polarization screening may have, playing a more preponderant role in the PCI effect observed in extended polymeric solid media. Our work offers insight into the generality of the PCI effect in systems of increasing complexity.

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Light Interferometer for Measurement of the Gravitational Behavior of Antimatter

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The QUPLAS (QUantum interferometry and gravitation with Positrons and LASers) experiment aims to test fundamental physical laws with antimatter by measuring the **Positronium (Ps) fall in the Earth's gravitational field**. Such measurement would represent a test of the **Einstein Equivalence Principle and the CPT symmetry** and is further motivated by the lack of information on antimatter behavior in the gravitational field.
The setup and techniques of the experiment involve three phases of production, preparation, and interference of the positronium beam. I will discuss the design, simulation and optimization of the **Large Momentum Transfer (LMT) Mach-Zehnder interferometer** [1] (see figure 1) used in the final stage of the experiment to reveal the influence of the Earth's gravitational field through the relationship that binds the phase shift of the wave function of Ps to the gravitational acceleration: $\Delta\varphi = k_{eff}\, gT^2$ [2]. By simulating the interferometer, it was possible to estimate its efficiency, contrast and signal acquisition times as well as determining fundamental operating parameters such as the size, shape and power of the laser pulses. These results will be shown in the exhibition.

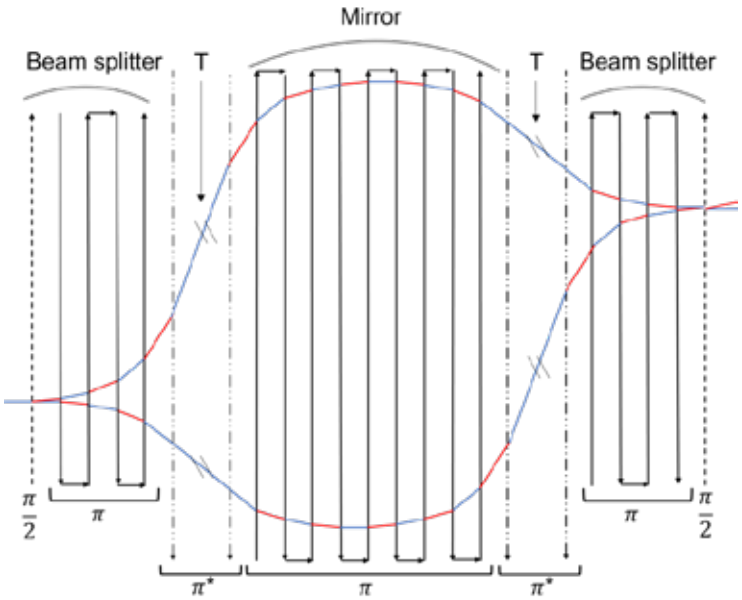

FIG. 1: Scheme of the light Interferometer. The Ps beam entering the apparatus will propagate according to a laser-driven Mach-Zehnder scheme, in order to acquire a phase induced by the gravitational field. The overall momentum transfer is given by the sum of all the pulses.

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IMPLEMENTATION OF SOFT X-RAY SPECTROSCOPY BEAMLINE BASED ON HHG FOR THE STUDY OF ULTRAFAST DYNAMICS IN ADVANCED MATERIALS

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With conventional semiconductors facing a shortage lately, the need for alternative resources grows stronger. One potential candidate is $3D$ perovskites whose interesting properties – e.g., low exciton binding energy [1], defect tolerance [2], large polarons [3] - constitutes them perfect candidates for light-harvesting devices [4].

Ultrafast soft X-ray spectroscopy allows studying light-matter interaction with an unprecedented temporal and spatial resolution, with the further advantage of being element-selective and oxidation- and spin-state specific. As such, we plan to investigate charge transfer dynamics in $3D$ perovskites with time-resolved Near Edge X-ray Absorption Fine Structure (NEXAFS) at the few femtosecond time scale, to unveil the role of the samples' constituents. Pump-probe spectroscopy is one of the most common experimental schemes for these types of measurements. In summary, a first pump pulse excites the sample, then the evolution is probed by a second time-delayed pulse. Hence, innovative experimental set-ups that focus on broadband detection, high dynamic range, and sensitivity have become a necessity in the field of ultrafast dynamics.

High order harmonic generation of femtosecond laser pulses interacting with noble gases has become a popular table-top source of broadband coherent XUV radiation throughout the years. By implementing a microfluidic device instead of the trusted gas-jet configuration, we obtained an extended energy cut-off, and a higher generation yield [5]. Furthermore, an integrated solution for filtering IR radiation under vacuum has been investigated. High vacuum systems were also realized for the manipulation, detection, and characterization of the generated XUV light.

However, all-optical techniques have huge untapped potential, given that conventional spectrometers are characterized by limited spectral ranges (either low or high-energy photons), and a lack of polarization characterization which excludes the studies of magnetic materials and biologically relevant molecules. Therefore, an innovative detection scheme was realized in our laboratory to surmount these limitations.

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Observing Superfluid Current Through a Dissipative Quantum Point Contact

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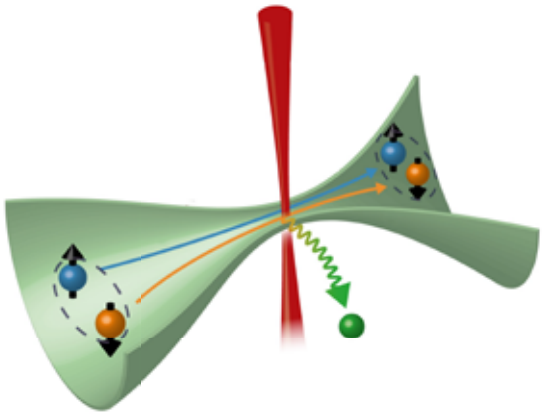
We experimentally and theoretically investigate the robustness of fermionic superfluidity to spin-dependent dissipation in a unitary Fermi gas. With a focused laser resonant with one of the two spin states, we introduce a controllable particle loss at a quantum point contact connecting two superfluid reservoirs. We measure the influence of the dissipation on the superfluid flow between the reservoirs, characterized by a non-Ohmic current-bias relation due to multiple Andreev reflections (MAR). A mean-field model in the Keldysh formalism qualitatively reproduces our observations, showing that there is no critical dissipation strength where the supercurrent vanishes. Instead, it decays smoothly with increasing dissipation while the current-bias relation approaches an Ohmic scaling, indicating a surprising robustness of MAR. Our current work extends to pure spin transport under local dissipation. These results are relevant for dissipative engineering of transport properties and understanding dissipative non-equilibrium superfluid systems.



Experimental concept: we measure superfluid current between two reservoirs of spinor (blue and orange) unitary Fermi gas through a quantum point contact (short 1D channel). A tightly focused resonant laser (red) at the contact transfers spin down (orange) into a third state (green), inducing dissipation.

Laser cooling of AlF molecules

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Aluminium monofluoride (AlF) offers unique opportunities for direct laser cooling of molecules. The "closed shell" structure of the electronic ground state results in a chemically stable and deeply bound molecule. The $A^1\Pi \leftarrow X^1\Sigma^+$ laser cooling transition is extremely strong, highly vibrationally diagonal and in the deep ultraviolet, allowing efficient and rapid optical cycling and the generation of large radiation pressure forces. In addition, the spin-singlet nature of the ground and excited states means that all Q(J)-lines are rotationally closed, in contrast to the spin-doublet molecules laser cooled thus far [1, 2].

We demonstrate the benefits of these molecular properties in experiments, both by producing the molecules with high efficiency, and with the first experiments laser cooling AlF. We generate AlF in a pulsed cryogenic buffer gas source with more than 10^{12} molecules per steradian per shot, and utilise the reaction between Al and AlF_3 to generate a continuous thermal AlF beam with a total brightness of 6×10^{14} molecules per steradian per second. These molecular beams are then subsequently laser cooled in one dimension with blue-detuned optical molasses, an important step towards magneto-optical trapping.

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Apparatus For Creating and Studying a Bose-Einstein Condensate of CaF Molecules

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Dipolar molecular gases can be used to study many-body quantum systems with long-range interactions. We aim to create a quantum degenerate gas of CaF and explore the behaviour of this strongly dipolar quantum gas, both in bulk and in a lattice.

We are building the apparatus shown in Fig.1. A beam of calcium monofluoride (CaF) molecules is created using a cryogenic buffer gas source [1], collimated using a combination of a magnetic lens and transverse laser cooling, and then slowed to low speed by the radiation pressure of a counter-propagating laser beam. The slow molecules are then captured and cooled in a magneto-optical trap [2]. From here, the molecules will be loaded into an optical dipole trap [3] in the presence of a molasses which is capable of cooling the molecules to 5 μK [4]. Evaporative cooling will then be used to increase the phase-space density towards BEC. To suppress reactive and inelastic collisions, a static electric field at 22kV/cm will be applied to create a potential barrier that prevents the molecules from getting too close [4] and also enhances elastic collision rates. We predict that it is possible to reach BEC in 0.7 s, with 10^5 molecules at 250 nK and a density of 1.4×10^{13} cm^{-3}. The molecular condensate will be an inspiring platform for a variety of research, especially the quantum simulation of strongly-interacting many-body quantum systems.

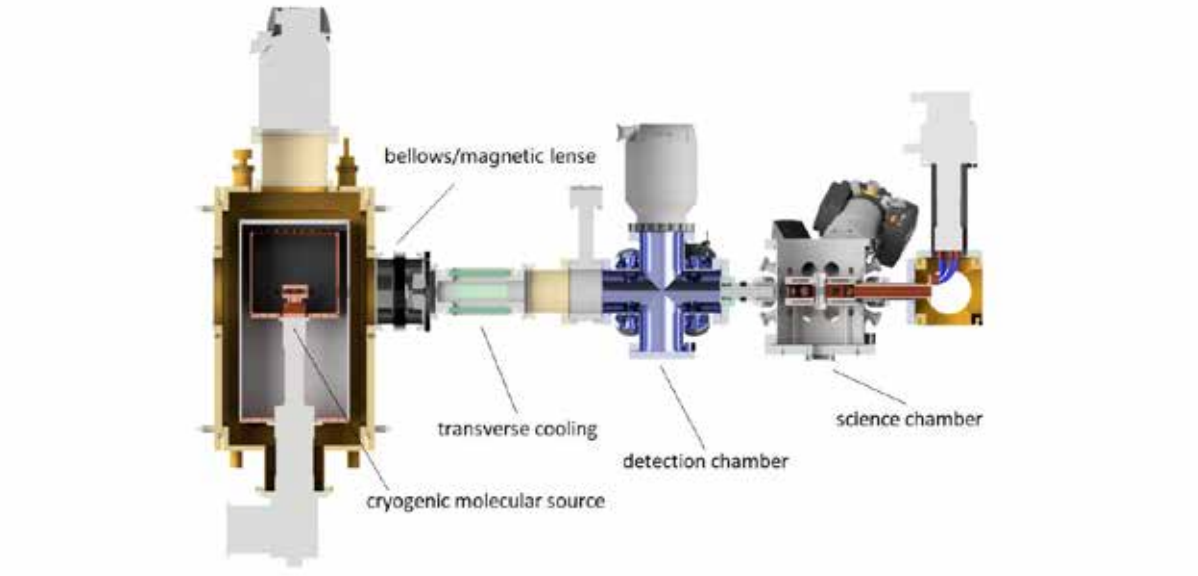

FIG. 1: The experiment setup.

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Radiative Cooling of Polyyne Anions: C_4H^- and C_6H^-

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The time-dependent photodetachment action spectra of the linear hydrocarbon anions C_4H^- and C_6H^- are investigated using the cryogenic electrostatic ion storage ring DESIREE. Radiative cooling characteristics of the ions on the millisecond to second timescale are probed by monitoring changes in the spectra as the ions cool by spontaneous infrared (IR) emission. A simple harmonic cascade (SHC) model is used to model the cooling processes. The cooling rates, extracted using Non-negative Matrix Factorization (NMF), are fit with 1/e lifetimes of 19 ± 2 s and 3.0 ± 0.2 s for C_4H^- and C_6H^-, respectively. For C_4H^-, the adiabatic detachment energy is determined from the cold ions' photodetachment spectra to be 3.45 ± 0.02 eV. The photodetachment spectrum and the ultraslow radiative cooling dynamics interpreted in the present work provide important data for understanding the thermal cooling properties of linear hydrocarbon anions and for refining the formation and destruction processes of these anions in astrochemical models.

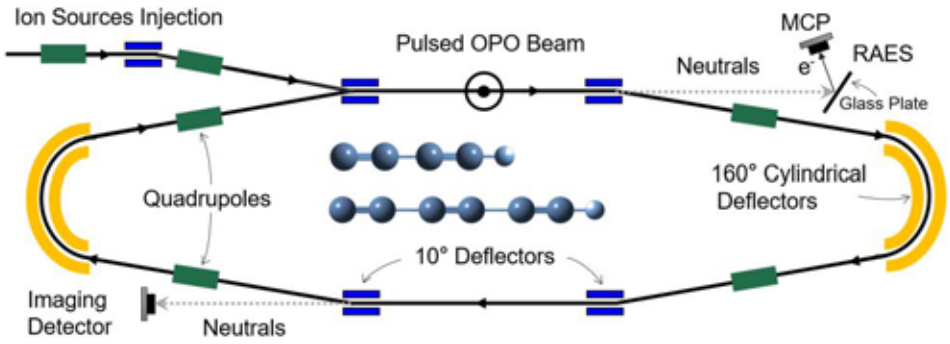

FIG. 1: Schematic drawing of the DESIREE ion storage ring. The OPO laser beam interacts perpendicularly with the ion beam on the RAES detector side. Neutral products formed through photodetachment along the traight section are detected by the microchannel plate (MCP) detector.

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New production scheme of HCI using antiprotonic atoms

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Access to a variety of highly charged ions is crucial for fundamental research and for technological applications. However, not all isotopes can be accessed with the existing production paths. Therefore, in order to provide an alternative production mechanisms of either difficult to obtain radioisotopes or HCI's of short-lived isotopes, new approaches are needed.

We suggest that many species of HCI can be accessed using antiprotonic atoms. They are atoms in which one electron is replaced by an antiproton ($\bar{p}$). The lifetime of these atoms depends on the relaxation of the antiproton and ultimately annihilation with the nucleus matter of the atom. The annihilation happens on the surface and with little recoil momentum of the nucleus. Pions (or more rarely, kaons) that are produced in the annihilation can then interact with nucleus matter creating new isotopes, already in HCI state.

We have studied in detailed simulations done using GEANT4 code the annihilation of very low energy $\bar{p}$ on atoms at rest. We have explored the process for light, medium and heavy atoms. The simulations gave as insights on the produced fragments and unstable particles which could be traced inside the simulation code giving their mass, momentum and charge. According to this simulation, by starting the process with very low energy $\bar{p}$ captured by atoms at rest, it is possible to create isotopes^{Z+} with energies which enable their capture for further studies and manipulations, which could not be achieved with previous methods. The production scheme of HCI could benefit further if combined with the pulsed production of cold protonium [1] atoms (a bound state of a proton and an antiproton) where ns control of the formation time can be achieved via a charge exchange reaction happening between highly excited Rydberg state of atoms and co-trapped antiprotons. The results of our simulations show that it is possible to create and trap isotopes that were previously unobtainable.

The work was funded by Warsaw University of Technology within the Excellence Initiative: Research University (IDUB) programme and the IDUB-POB-FWEiTE-1 project grant.

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High-dimensional Time-Space Crystalline Structures And Their Topological Properties

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Regular space crystals are described by a spatially periodic distribution of particles observed at a fixed moment of time. To form time crystals [**1**, **2**], the roles between time and space are interchanged. In this case the periodicity is observed in time by fixing a position in space and measuring the periodic detection of particles during the experimental time frame. Time crystal behavior can emerge spontaneously in many-body systems and can also be engineered by suitable external time-periodic driving. This allows for a realization of a variety of condensed-matter phenomena in the time domain [**3**, **4**].

In this work, we demonstrate the notion of time-space crystalline structures (TSCS) which merge the ideas of time and space crystals to form systems that are both temporally and spatially periodic [**5**]. Starting with a particle in a one-dimensional periodic potential, an external periodic and resonant driving can be used to engineer a crystalline time structure at each potential well of the spatial lattice thus effectively forming a two-dimensional TSCS. This allows us to construct a system where each spatially orthogonal one-dimensional periodic potential comes equipped with a periodic structure in time. For a three-dimensional lattice with a proper choice of driving this leads to a six-dimensional TSCS. These structures pave the way towards investigation of higher-dimensional condensed-matter phases, including studies of their topological properties. We show that in time-space crystals one can perform topological charge pumping [**6**] along both the temporal and the spatial dimensions, which in turn provides a means of exploring the quantum Hall effect in higher dimensions [**7**].

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A Strongly Interacting Fermi Gas Dispersively Coupled to Light

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Combined quantum-gas cavity systems offer the possibility to implement, simulate, and experimentally realize fundamental solid-state Hamiltonians, along with non-equilibrium many-body phenomena in open quantum systems, which go beyond conventional condensed-matter scenarios [1]. In our experiment, we combine a quantum degenerate, strongly interacting Fermi gas of Lithium 6 with a high finesse optical cavity [3], therefore strongly coupling atoms [2] as well as atom pairs to light [4]. By driving the cavity in the dispersive regime, we observe a Kerr non-linearity originating from the optomechanical coupling of photons with the density fluctuations of the strongly interacting Fermi gas. I will discuss the measurement of this few-photon non-linearity as a function of interaction strength in the BEC-BCS crossover and its connection to the strength of pair correlations [5]. Through the addition of a laser beam pumping the atom-cavity system transversally to the cavity axis, we engineer photon-mediated interactions between atoms. Recently, the crossing of the superradiant phase transition for a non-interacting Fermi gas was observed for sufficently strong pump strengths [6]. I will report on the first experimental realization of self-organization of strongly interacting Fermions. This opens up the possibility of studying the competition between long and short-range interactions in the BEC-BCS crossover.

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