

ECAMP 15

Monday, June 30, 2025 - Friday, July 4, 2025



Book of Abstracts

**15th European Conference on Atoms, Molecules and
Photons**

June 30 - July 4, 2025

Congress Center Innsbruck

*Editors: Viviane Schmidt, Eric Endres, Robert Wild,
Roland Wester*

Welcome

Dear Participants,

it is our great pleasure to welcome you to Innsbruck, urban city in the mountains and informal capital of the Alps, for the 15th European Conference on Atoms, Molecules and Photons. Since its first edition in 1981, the triennial ECAMP conference series arrives for the first time in Austria, after Vilnius (2022), Florence (2019), and Frankfurt (2016).

A rich and diverse scientific program awaits you with 9 plenary talks, 54 invited talks, 32 hot topic talks, and 248 poster presentations. In addition to the well established topics on collisions, spectroscopy, ultrafast dynamics, clusters, ultracold gases, and fundamental physics, this ECAMP edition offers for the first time current research in quantum technologies, quantum optics, cavity QED, and quantum information. In the International Year of Quantum Science and Technology, the scope of the conference embraces novel avenues taken within our Atomic, Molecular and Optical Physics community.

We hope you will enjoy the uniqueness of the city of Innsbruck and its magnificent natural surroundings as much as the scientific conference itself. We wish you a great ECAMP experience.

Roland Wester

Chair of the Local Organizing Committee

Alicia Palacios

Chair of the AMOPD Board



Organizers

Scientific Committee

Alicia Palacios – Chair
 Iva Brezinova – Vice-chair
 Paola Bolognesi (EPS-EAC)
 Francesco Cataliotti
 Mathieu Gisselbrecht
 Rosario Gonzalez-Ferez (EGAS)
 Saïda Guellati-Khelifa
 Till Jahnke
 Nikolai Kolachevsky
 Daniela Rupp
 Stefan Schippers (ICPEAC)
 Karolina Slowik
 Frank Stienkemeier (CMPS)
 Hugo van der Hart
 Roland Wester



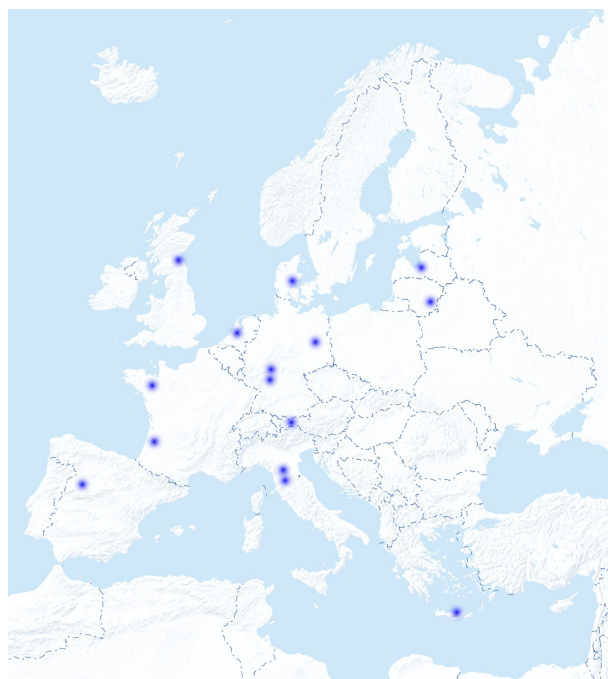
Local Organizing Committee

Roland Wester – Chair
 Francesca Ferlaino
 Hanns-Christoph Nägerl
 Katrin Erath-Dulitz
 Robert Wild
 Eric Endres



Previous ECAMPs

1981	Heidelberg
1985	Amsterdam
1989	Bordeaux
1992	Riga
1995	Edinburgh
1998	Siena
2001	Berlin
2004	Rennes
2007	Heraklion
2010	Salamanca
2013	Aarhus
2016	Frankfurt
2019	Florence
2022	Vilnius
2025	Innsbruck



mapswire.com - CC-BY 4.0

Sponsors

We thank our sponsors:



Public evening lecture



We are delighted that Prof. Rainer Blatt will give the public lecture at ECAMP15.

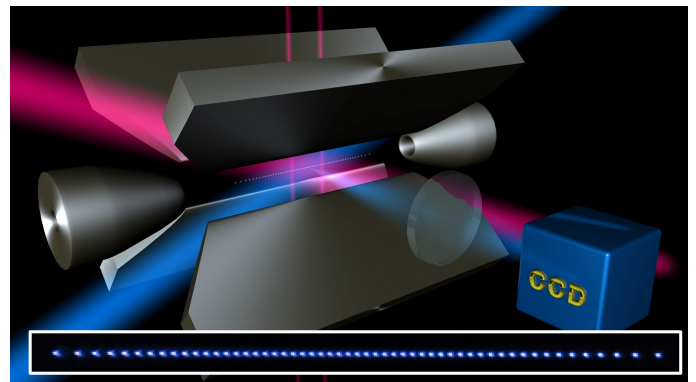
Rainer Blatt is a leading researcher in the field of quantum physics at the University of Innsbruck and the Institute for Quantum Optics and Quantum Information (IQOQI). He is internationally renowned for his pioneering work on quantum computers based on trapped ions.

The Quantum Way of Doing Computations

Thursday, July 3, 2025 at 19:30

Abstract

We are on the verge of a new era in computing, powered by the bizarre yet powerful world of quantum physics. Scientists are learning to control individual atoms, using them as the building blocks for potentially powerful computers. In this talk, we delve into how these “quantum machines” work, specifically focusing on how we trap and manipulate ions as quantum bits. We will explore the types of problems quantum computers can solve, and discuss the exciting challenges and possibilities that lie ahead in this rapidly developing field.



Contents

Welcome

Plenary Talks

Attosecond light pulses for studying electron dynamics	20
Quantum networking resources and applications	20
A molecular bond between ions and Rydberg atoms	20
The Secret Life of Catalysts: Operando Spectroscopy and Microscopy as Powerful Tools for Mechanistic Understanding	20
Tests of fundamental symmetries using antihydrogen: the ALPHA experiment at CERN	20
Negative Ions - Fragile Quantum Systems	21
Lighting a path for quantum metrology and fundamental physics	21
Dynamics in Atomic and Molecular Physics in the x-ray domain	21
Shedding Light on Nuclear Spins: Through the looking-glass	21

Spectroscopy 1

Statistical Analysis of Raman Spectra of Biofuels: The Case of Myristic Acid Conformers	22
Molecular conformations in floppy chiral systems probed by Photoelectron Circular Dichroism (PECD)	22
Towards trapping cold hydrogen molecules	22
Liquid-jet Velocity Map Imaging	23
Core-level electron transfer mediated decay in microhydrated pyrimidine	23

Ultrafast 1

Ultrafast preparation and detection of entangled atoms using a COLTRIMS reaction microscope	23
X-ray superfluorescence	24
Shaping light in 3D to twist electrons on an ultrafast timescale	24
Measurement and control of interactions in bosonic optical clocks	24
Entanglement-Enhanced Atomic Gravimeter	25

Collisions 1

Controlled collisions of molecules and ions	25
Reactive collisions of oxygen atoms with aromatic compounds in crossed-beam experiments	25
The Mutual Neutralization of Hydronium and Hydroxide.	25
Quantum State Selection and Laser Cooling Systems for Studying Collisions and Reaction Dynamics at Low Temperatures	26

Quantum 1

Rethinking Resonance Fluorescence: Fundamental Insights and Emerging Quantum Technologies	26
Protecting collective qubits	26
Observation of anomalous information scrambling in a Rydberg atom array	27

Large Systems 1

Exploring quantum Hall physics with ultracold dysprosium atoms	28
Electronic Quantum Dynamics in Helium Droplets traced by Coherent Diffractive Imaging	28
Ultrafast relaxation processes in photoexcited He nanodroplets	28
Peptide bonds formation in clusters of amino acids in the gas phase induced by ionizing radiation.	28
Cryogenic single nanoparticle mass spectrometry	29

Quantum 2

Quantum interfaces with ions and nanoparticles	29
Non-local quantum many-body systems	29
Building a quantum network one photon at a time	30
Self-Assembled Chains and Solids of Dipolar Atoms in a Multilayer	30
Stabilisation of spin mixtures and bound state spectroscopy in dipolar gases	30

Collisions 2

Ion processing of astrophysically relevant molecular systems	30
Electron collisions with internally cold molecular ions in the Cryogenic Storage Ring	31
Cooling and colliding oppositely charged ions	31
Laser-induced ionization triggers correlation-driven charge migration	31
Ultrafast correlation dynamics during high-harmonic generation in multi-electron atoms	32

Fundamental 1

Precision Spectroscopy in Ion Coulomb Crystals and Search for New Physics	32
High-resolution spectroscopy of molecular hydrogen ions	32
Trapped ions in optical tweezers	33

Ultracold 1

Exploring the Roles of Nuclear Spins, Quantum Coherence, and Entanglement in Ultracold Chemistry	33
Ultracold highly magnetic and polar molecules for quantum simulation and new physics search	33
Testing fundamental physics with ultracold molecules	33

Ultrafast 2

Attosecond and few-femtosecond electron dynamics in photoexcited and photoionized organic molecules	34
Controlling entanglement and the forces on the nuclei with atto and few femto-second pulses	34
Watching a molecular bond break	34

Ultrafast 3

Attosecond electron dynamics in solutions	35
X-ray induced Coulomb explosion images quantum fluctuations and reaction dynamics in complex molecules	35
Generating quantum entanglement using intense XUV-pulses from free-electron lasers	35
Spectroscopic measurements of the Rydberg-surface Casimir-Polder Interaction	36
Advances in High-Mass Matter-Wave Interferometry	36

Spectroscopy 2

High resolution single molecule spectroscopy in a cryogenic ion trap	37
Cavity-Enhanced Dispersive Interaction of Cold Atoms with an Optical Frequency Comb	37
Spatio-temporal tailored attosecond light pulses for exploring ultrafast localized phenomena	37
Coherent nonlinear four X-ray photon interaction with core-shell electrons	37
Measurement of Single Photon Photoelectron Elliptical Dichroism of Electrosprayed Anions	38

Ultracold 2

Exploring Rydberg Atom Interactions Near Optical Nanofibres	39
Hydrodynamics in an Ultracold Dipolar Gas	39
Microscopy of strontium Bose- and Fermi-Hubbard systems	39
A cavity-microscope for micrometer-scale control of atom-photon interactions	40
Collective light scattering in an array of dysprosium atoms	40

Ultracold 3

Quantum continuous time crystals in neutral-atom arrays	40
Thermal melting of a vortex lattice	40
From Bose polarons to quantum droplets of light	41

Quantum 3

Quantum control of massive mechanical objects	41
Non-Hermitian Skin Effect for Photon Pairs Interacting with Atom Arrays	41
Dissipative phase transitions with one and many atoms in cavities	41
Ultrafast imaging of ytterbium tweezer arrays	42

Collisions 3

Quantum resonances in cold collisions	42
Cold and controlled collisions using tamed molecular beams	42
Electron Diffraction Imaging of Molecules via Ionization by Compton Scattering	43
Convergent Close-Coupling Approach to Electron-Impact Dissociative Excitation and Ionisation of H_3^+	43

Quantum 4

Many-body theory and calculations of positron binding, scattering and annihilation in polyatomic molecules	44
Quantum Optics with Rydberg Excitons	44
Adiabatic echo protocols for robust quantum many-body state preparation	44
From Quantum Statistics to Work: The Pauli Engine and Beyond	44
Quantum-enabled Rydberg atomic polarimetry of radio-frequency fields	45

Fundamental 2

Nuclear-solid interactions in Thorium-229	46
Testing quantum electrodynamics in extreme fields using helium-like uranium	46
Vortices in a dipolar supersolid and single erbium atoms in optical tweezers	46
Collective effects in thermometry and cooling of trapped ions	46

Ultrafast 4

Generation of optical Schrödinger "cat" states using intense laser-matter interactions and applications in non-linear optics	47
Two-dimensional sub-wavelength topological lattices for dark-state ultracold atoms	47

Interplay of locally chiral rotational and electronic currents in chiral molecules	47
Femtosecond timed imaging of rotation and vibration of alkali dimers on the surface of helium nanodroplets	48

Spectroscopy 3 / Ultracold 4

A pedestrian route to modeling atomic processes	48
Liquid-jet photoelectron spectroscopy of aqueous solutions: Electron scattering, electronic structure and work functions	49
Observation of a new, regular series of highly doubly excited states in Sr	49
Collisional excitation of interstellar chloronium: accurate rate coefficients with astrophysical applications	49

Young Scientist Award

Advancing cold molecular ion spectroscopy using helium nanodroplets	50
---	----

Poster Session A

Determination of Desorption Energies in Dispersion-dominated Complexes: Role of Nitrogen Substitution and Functional Group	51
Airy offset of velocity imaging-based electron spectrometry	51
Light absorption and emission processes involving charge transfer states of weakly-bound molecular ions in noble gas mixture plasmas	51
Electron transfer processes and the formation of solvated dielectrons by UV excitation in sodium-ammonia clusters	52
Photoabsorption Spectroscopy using adQTB Dynamics	52
Single Photoionization of vinylcyanoacetylene and methacrylonitrile in Astrophysical Objects	52
Photodesorption of CO ices: Rotational and translational energy distributions	53
New Spectral Features on Two-Dimensional Optical Spectra arising from Quantum System-Bath Interactions: Implications and Potential Applications	53
The survival mechanisms of dipeptides to space environmental conditions	54
Multiplatform computing of oscillator strengths and transition probabilities in Os V	54
Bayesian methods for quantum logic spectroscopy	54
Structural Characterization of Interstellar Water Ice Analogues: Optical and Morphological Evolution with Deposition Conditions	55

Photofragmentation of dAMP- in a cryogenic ion trap	55
Experimental Oscillator Strengths For Forbidden Lines IN Fe II	55
Luminescence and scintillation properties of zinc-silicate glass ceramics	56
Coherent nonlinear four X-ray photon interaction with core-shell electrons	56
Erosion of the lunar surface by solar wind ions	57
Ion–molecule reactions of acetylene inside helium nanodroplets: Formation of cationic benzene and other covalently bound hydrocarbons including PAHs	58
Impact of a smoothing parameter in breast radiotherapy planning	58
Reactivity of Sea Salt Cluster Ions with Atmospherically Relevant Organic Acids in the Gas Phase	58
Apparatus for preparing conformationally pure gas-phase biomolecular clusters	59
Anyonization of bosons	59
Bloch Oscillations of a Soliton in a 1D Quantum Fluid	59
Optical excitation and stabilization of ultracold field-linked tetratomic molecules	60
Ultracold Coherent Control of molecular collisions at a Förster resonance	60
Combining atomic ensembles with single atoms to realize collectively enhanced detection using EIT	61
Dipolar Supersolids as a Platform for Tunable Josephson Junctions	61
All Optical Formation of Bose-Einstein Condensate near Dielectric Surface	61
Interactions between metastable triplet-state helium dimers	61
High fidelity control of a many-body Tonks-Girardeau gas with an effective mean-field approach	62
Barium Fluoride Deceleration Using Temporary Ionization	62
Towards the Simulation of Complex Models of Quantum Magnetism with Electromagnetic Dipoles	62
Two-Photon Optical Shielding of Collisions Between Ultracold Polar Molecules	63
High-fidelity quantum logic state detection of single trapped molecular ions	63
Structure, stability and superfluidity of Bose-Bose bulk mixtures and droplets in quasi-2D confinement and optical lattices	64
Modeling weakly bound few-body systems of ultracold quantum mixtures	64
Collective effects in thermometry and cooling of trapped ions	64
Vortices in a dipolar supersolid and single erbium atoms in optical tweezers	64
Role of electron-impact charge transfer excitations of molecular and quasimolecular ions in the relaxation processes in noble gas mixture plasmas	65
Photoionization of neutral PAHs in space - New lab data on photoelectric heating	65

Electronically resolved excitation in proton collisions with hydrogen molecules	66
Resonances and dissociative dynamics of iron tetracarbonyl acrolein	66
Hydrogen Sticking Dynamics on Graphene	67
Source of negatively charged ions for matter-antimatter interaction experiments	67
Impact parameter and kinematic information for differential ionization of argon by positron and electron impacts	67
Commissioning of the Transverse Free-Electron Target at the Heavy-Ion Storage Ring CRYRING@ESR	67
Associative ionisation of $H(1s) + H(ns)$: a semi-classical description	68
Crossed-beam Scattering Dynamics of Atomic Nitrogen Ions with Carbon Dioxide Molecules	69
Electron and Ion Induced Reactions with Chlorpyrifos Molecules	69
Dissociative positronium attachment in halogen gases	69
Gas phase collisions of O^+ ions in ^4S and ^2D states with molecular moieties of space-relevant polymers	70
C_{60}^+ collisions with low-energy electrons at the Cryogenic Storage Ring	70
Convergent Close-Coupling Approach to Electron-Impact Dissociative Excitation and Ionisation of H_3^+	71
From megabarns to attoseconds: How to relate the cross-section with the time delay	71
Spin and Orbital Angular Momentum in Attosecond Pulses of Light	71
Amplification of spontaneous emission from doubly excited He atoms	72
Adiabatic alignment of alkali dimers on the surface of helium nanodroplets	72
Verifying Fano's propensity rules by interfering photoelectron wavepackets of different parities	73
Correlated Strong-Field Double Ionization	73
Effect of Laser Repetition Rate on Electron Emission from Tungsten Nanotip	73
Strong electron-electron-nuclei correlations in multiphoton single and double ionization	74
The role of dephasing in solid-state high harmonic generation	75
Modelling of photoionization time-delays in iodine-containing molecules with scalar relativistic effects	75
Photo-modified birefringence of low thermal noise crystalline AlGaAs mirror coatings for ultrastable lasers	75
Multi-species cold-atom interferometry for inertial measurements	76
Coupled atom-cavity systems for quantum-enhanced metrology: adiabatic elimination of the cavity mode beyond the leading order	76
Towards the Assembly of YbCaF	76
Temperature Dependence of ac Stark Shift in a Vapor Cell Rb Atomic Clock	77
Status of Rb Two-Photon Optical Clock with a Chip-Scale Vapor Cell at KRISS	77

Floquet Theory of Sequential Bragg and Bloch Oscillation Based Large Momentum Transfer	77
Direct comparison of polarizability measurements with a dual-species ion clock	78
Collective Quantum Phenomena	78
Rapid and Robust Hyperfine Qudit Gates in Trapped Neutral Atoms	78
Hot Schrödinger Cat States	78
Unconventional Phonon blockade effect in a coupled nanomechanical system quadratically coupled to a two-level system	79
Full-stack neutral-atom quantum computing with ^{85}Rb	79
Reconstruction of Quantum Gates using Quantum Process Tomography	79
Utilizing the center of mass for sensing magnetic fields and gravity in a cold atom cavity QED system with magnetic trapping	80
Quantum Annealing for Combinatorial Optimization and Many-Body Physics: Room Scheduling and Z_2 Spin Liquid	80
Environment-Enhanced Single-Photon Absorption in a Nanoring of Dipole-Coupled Quantum Emitters	80
Protecting collective qubits	81
Quantum Correlations in UV Dual-Comb Spectroscopy	81

Poster Session B

Quantum Monte Carlo study on positron binding to atomic anion dimers	82
Cyclic C_4^+ as the carrier of diffuse interstellar band at 503.9 nm	82
Characterization of the spectral signal of the double-well broad potential curve of NaH D state	82
Electron-Photon Coincidence Measurements at the Syn- chrotron Facility MAX IV during TRIBs operation mode	82
Mid-infrared frequency comb spectroscopy in uniform supersonic flows: A look into vibrational excitation in Laval nozzles	83
Photoionisation, Rayleigh, and Raman scattering cross sections for the hydrogen molecule and its ion	83
Monochromatic source of ions and electrons for nanosciences	83
High resolution spectroscopy of molecules confined in gas cells of sub-wavelength thickness	84
Comb-based Fourier-transform cavity-ringdown spectroscopy	84
Chirality induced spin polarization in one-photon ionization by circularly polarized light	85
Multi-platform theoretical calculations of oscillator strengths and transition probabilities in the Yb I isoelectronic sequence (Ta IV - Pt IX) for nuclear applications	85
The interplay of bulk- and microviscosity effects on BODIPY-based molecular sensors	86

Towards deterministic ionization, loading, and sympathetic cooling of molecular ions for quantum logic spectroscopy	86
Single and double ionization of pyridine and pyridine clusters	86
Internal decay processes in electron-rich symmetric dimer anions: An experimental probing using trapped ions in an Electrostatic ion-beam trap (EIBT)	86
Ground and First Excited States of the NaSr Molecule: Experimental and Theoretical Study	87
Spectroscopic Studies of Cold, Trapped Negative Ions in Radiofrequency Multipole Traps	87
High-Fidelity Individual Addressing of Single Atoms in Quantum Registers at Three-Photon Laser Excitation of Rydberg States	88
Electron Diffraction Imaging of Molecules via Ionization by Compton Scattering	88
The features of binding of two multi-charged meso-porphyrins to nucleic acids	89
Highly oriented pyrolytic graphite chemical bonding structure after gallium implantation	89
The primary steps of ion solvation in helium nanodroplets	89
Cryogenic single nanoparticle mass spectrometry	90
Collisional effects in the ultracold Rb-Hg system	90
Measurement of atom-surface interactions in evanescent light filed by cold atomic fountain	90
Excitations of a binary dipolar supersolid	91
Dipole-Mode Spectrum and Hydrodynamic Crossover in a Resonantly Interacting Two-Species Fermion Mixture	91
Dynamical quasicondensation in the weakly interacting Fermi-Hubbard model	92
The moving Fermi polaron	92
Laser slowing of Aluminium-monofluoride in the deep ultraviolet	92
Coherent control, state preparation and readout of polyatomic molecular ions via Quantum Logic Spectroscopy	92
Unitary Transformations using Robust Optimal Control on a Cold Atom Qudit	93
Spatially-resolved spin manipulation and readout of individual ultracold molecules in an optical lattice	93
Optical creation and manipulation of localised vortices in two-component Bose–Einstein condensates	93
Creation of ultracold Bosonic $^{39}\text{K}^{133}\text{Cs}$ Molecules in the rovibrational ground state	94
Density functional studies of vortices in rotating squeezed Bose-Bose mixtures	94
Prospects for Laser Cooling BN^-	94
Collective light scattering in an array of dysprosium atoms	95
Self-Assembled Chains and Solids of Dipolar Atoms in a Multilayer	95
Towards highly polar CsAg and KAg ground state molecules	95

How rotation shapes the decay of diatomic carbon anions	96
Atomic cascade computations for astro and plasma physics	96
Angle-resolved spectroscopy of secondary electrons from surfaces emitted by highly charged ion impact	96
Does electron emission in highly charged ion collisions with surfaces occur above the surface or below?	97
Electron collisions with liquid microjets: spectroscopy and reactivity	97
State selective charge-exchange cross sections in collisions between Cq^+ ions with sodium atoms	97
Many-Body Theory Calculations of Positron Binding to Picolines	98
Experimental & theoretical cross sections for single & double ionization of open-4d-shell ions Xe^{12+} to Xe^{14+} by electron impact	98
Ternary association of H_3^+ with H_2 : effect of rotational excitation	98
Caesium photoionization for monochromatic electrons source for surface electron microscopy	99
Experiments on Three-Body Association of Noble Gases in an RF Multipole Ion Trap	99
Atomistic Computer Simulations of $Fe(CO)_5$ Fragmentation Dynamics on a Substrate	100
Dissociative electron attachment as a mechanism for formation of negative molecular ions in the interstellar medium	100
The Mutual Neutralization of Hydronium and Hydroxide	100
Attosecond magnetic pulses emerging from ring-current gates	101
Ionization-induced proton-transfer dynamics in formic acid dimer	101
Autodetachment and autofragmentation in anionic species	101
All-optical coherent control of chiral electronic transitions for highly enantioselective photochemistry	101
Ultra-fast nonlinear optical response of chiral molecules with a focus on conformer sensitivity	102
Modelling sequential ionisation within time-dependent R-Matrix Theory	102
Excited-State Dynamics of Pyrazine and the Role of Electronic Coherences	103
Electronic coherences in molecules with XFAIMS	103
Methods for analysing photoelectron momentum distributions from attosecond light pulses	103
New magic wavelength for Sr clock transition	104
Squeezing-enhanced accurate differential sensing under large phase noise	104
Hydrogen atom diffraction through free-standing single-layer graphene	105
Cold Rydberg Strontium Atoms for the Thermometry of Optical Lattice Clocks	105
Measuring the Electron's Electric Dipole Moment Using Ultracold YbF Molecules	105
Optical Frequency Division for Ultra-Stable Microwave Generation and Remote Clock Referencing	106

Molecular spectroscopy in the THz range under sub-Doppler regime	106
The ground state hyperfine splitting in muonic hydrogen experiment (HyperMu) at PSI	107
Chip-scale Rydberg Quantum Electrometry	107
Stringent Tests of Theory via High Precision Measurements with Single Ions in the ALPHATRAP Experiment	108
A definition of the SI second based on several optical transitions	108
The Cumulant Expansion Approach: the Good, the Bad and the Ugly	108
Correlated vortex generation in coherent medium	108
Quantum Metrology in the Ultrastrong Coupling Regime of Light-Matter Interactions: Leveraging Virtual Excitations without Extracting Them	109
Triggered photons from an ion-mirror system	109
Quantum information processing and error correction in molecular rotation	109
Gravity in the Cavity: Cavity QED as a quantum simulator for cosmological perturbations	110
Development of ion trap technologies for studying mesoscopic quantum states	110
Progress toward Neutral Atom Array Processor	110
From Quantum Statistics to Work: The Pauli Engine and Beyond	110
2D Coulomb Crystal Vibrational Dynamics for Qubit Application	111

Poster Session C

Cold electronic spectroscopy of metal phthalocyanine cations	112
Quantum Optimal Control of Molecular Orientation	112
Photodetachment vibronic dynamics using nonlocal discrete-state-in-continuum model	112
Fourier-limited electronic transitions in surface-adsorbed quantum emitters	113
Laser spectroscopy of the X-A transition in CO ⁺⁺	113
Vibrational Induced Molecular Magnetism: A Theoretical Perspective	113
Highly oriented pyrolytic graphite chemical bonding structure after gallium implantation	114
Calculated absorption and circular dichroism spectra of TPPS4 molecular aggregates	114
Atomic data for Os VI spectral lines of interest to nuclear fusion research from independent computational approaches	114
Bottom-up Analysis of Ro-Vibrational Helical Dichroism	115

Testing strong-field QED to second-order in highly correlated berylliumlike Pb^{78+} by electron-ion collision spectroscopy	115
Multiple photoionization of singly charged lanthanum ions	116
Infrared absorption spectroscopy of single polyatomic molecular ions	116
Transition from Rabi Oscillations to Dynamic Interference seen in the Autler- Townes Doublet: A Multi-Peak Pattern Analysis	116
Experimental Characterization of All Vibrationally Excited States of the $X^+ \ ^2\Sigma_u^+$ Ground Electronic State of He_2^+	117
An Investigation into CMOS Sensors as Spatially & Spectrally Resolved Soft X-Ray Detectors for Laser Produced Plasma Imaging	117
Liquid-jet Velocity Map Imaging	118
Detection of surface magnetism by x-ray spectroscopy of hollow atoms	118
Theoretical investigation on positron binding properties in water clusters	118
Energy loss function of samarium determined from the reflection electron energy loss spectroscopy spectra	119
Tailoring optical response of atomic systems with low-dimensional nanoantennas	119
Long-Term Electrostatic Trapping of Multiply Charged Helium Nanodroplets in a Multi-Reflectron Time-of-Flight Device	120
Observation of many-body dynamical localization	120
Thermal fading of the $1/k^4$ -tail of the momentum distribution induced by the hole anomaly	121
Zero-Point-Energy Driven Isotopic Exchange of the $[\text{H}_3\text{O}]^-$ anion Probed by Mid-Infrared Action Spectroscopy	121
Laser cooling Rydberg molecules - He_2	121
Sunlight and the single atom - a photodetector for fundamental physics and daylight communications	121
Ab initio simulation of the interplay between an impurity and a measuring environment using ultracold atoms	122
Zeeman-Sisyphus deceleration of ultra-cold CaF molecules	122
Efficient loading of ultracold atoms into standing wave potential near dielectric surface	123
Josephson Oscillations in long ballistic channels	123
Cryogenic apparatus for quantum logic spectroscopy of polyatomic molecular ions	123
Universal momentum tail of identical one-dimensional anyons with two-body interactions	123
Topological transport properties of height modulated subwavelength barrier lattices	124
Light-Induced Losses and Pauli Suppression of Inelastic Collisions in a Sample of Trapped Bosonic Feshbach Molecules of $^{161}\text{Dy}^{40}\text{K}$	124
Interfacing Rydberg atoms with a high overtone bulk acoustic wave resonator in the GHz regime	124
Towards all-optical entangled BECs in microgravity	125

Tunable Field-Linked s-Wave Interactions in Dipolar Fermi Mixtures	125
Bosons in a 1D Quasiperiodic Optical Lattice studied via tVMC method	126
Construction and Characterization of a Ca Magneto-Optical Trap for Rydberg Physics	126
A cavity-microscope for micrometer-scale control of atom-photon interactions	126
Single and Double Ionization of Sn^+ and Sn^+ by Electron Impact	127
Negative Ion Chemistry Among Stars And Clouds: Molecular Processes In The Interstellar Medium	127
The quadrupole ion trap apparatus for ionization cross-section experiments	127
Electron collisions with molecular hydrogen for plasma-modelling applications	128
Cryogenic hybrid trapping of Ca^+ ions and OH molecules for cold ion-molecule reaction studies	128
The lifetime of a freely decaying hollow atom	128
Measuring ion-induced biomolecular fragmentation using a Velocity Map Imaging spectrometer	129
Electron-Induced Fluorescence of Carbon Monoxide	129
Transfer ionization dynamics in collisions involving light ions and helium atoms	130
Mutual neutralization reactions in collisions between pyrimidine cations and oxygen and chlorine atomic anions	130
Scattering studies between metastable neon and aligned ND_3	130
Mutual Neutralization with initial-state control	131
High rotational quantum states in spin orbit state selected charge transfer reaction	131
Electron-driven reactivity of molecular cations: from mechanisms to cross sections	131
Xenon photoionization in the vicinity of 4d giant resonance and Cooper minimum using an XUV-NIR pump-probe experiment at FLASH	132
Ionization Induced Dynamics	132
Real time observation of the formation of Li^+ -benzene complexes	132
Driving and Imaging Achiral-to-Chiral Transitions in an All-Optical Setup	133
RABBITT including Higher-Order Processes	133
First-principles evaluation of the complete HHG observable in solids	133
Partial-wave transitions in attosecond time delays and separability of Wigner delays	134
Ultrafast correlation dynamics during high-harmonic generation in multi-electron atoms	134
Femtosecond timed imaging of rotation and vibration of alkali dimers on the surface of helium nanodroplets	134
Magnetic field system for AQuRA transportable quantum clock	135
Reduced instability in a high-accuracy $^{115}\text{In}^+ / ^{172}\text{Yb}^+$ Coulomb crystal optical clock	135

Absolute quantum gravimeter and gradiometer for field applications	135
Optical clock spectroscopy with Sr ensembles in reconfigurable tweezer arrays	136
Searching for dark matter with a spin-based interferometer	136
Self-ordering, cooling, and lasing in an ensemble of clock atoms	136
Miniature quantum devices build of dipole coupled nano arrays of quantum emitters	137
Efficient computation of the classical bound of Bell correlation and prepare-and-measure witnesses in parallel environments	137
Non-Destructive Photon Number Measurement Using Quantum Phase Estimation	137
Efficient excitation energy transfer in a bio-inspired stacked nanoscale quantum emitter ring geometry	137
Demonstration of strong coupling of a subradiant atom array to a cavity vacuum	138
Landau polariton	138
Building scalable quantum computers at Oxford Ionics	138
Dissipation dilution in 3D direct laser written mechanical resonators	139
Creating and observing the hexadecapole moment in the fluorescence signal of the 87Rb D1 line: theoretical computations	139
Four-wave mixing in chip-scale Rb vapor cells in continuous wave mode	139
Progress toward an atomic-beam continuous-wave superradiant laser	140
Observation of anomalous information scrambling in a Rydberg atom array	141
An Apparatus for Controlling the Sr Clock Qubit	141

Schedule

Plenary Talks

Plenary 1: Monday, 9:00 - 10:00

Attosecond light pulses for studying electron dynamics

Anne L'Huillier

Department of Physics, Lund University, Sweden

When an intense laser interacts with a gas of atoms, high-order harmonics are generated. In the time domain, this radiation forms a train of extremely short light pulses, of the order of 100 attoseconds. Attosecond pulses allow the study of the dynamics of electrons in atoms and molecules, using pump-probe techniques. This presentation will highlight some of the key steps in the field of attosecond science, starting with the generation of high-order harmonics and continuing with the measurement of attosecond pulses. Applications in atomic spectroscopy will be presented.

Plenary 2: Monday, 14:00 - 15:00

Quantum networking resources and applications

Eleni Diamanti

Laboratoire d'Informatique 6 de Paris, Sorbonne Université, France

We discuss the main concepts, critical photonic resources, present efforts and challenges ahead aiming at the deployment of quantum communication networks at various stages of development, with both terrestrial and satellite links at a national and global scale. We present examples of applications of such networks spanning from ultrasecure communication to advanced cryptographic and communication protocols in distributed architectures.

Plenary 3: Tuesday, 9:00 - 10:00

A molecular bond between ions and Rydberg atoms

Tilman Pfau

5. Physikalisches Institut, Universität Stuttgart, Germany

Atoms with a highly excited electron, called Rydberg atoms, can form unusual types of molecular bonds. The bond differs from the well-known ionic and covalent bonds not only by its binding mechanism, but also by its bond length ranging up to several micrometers. We report the observation a new type of molecular bond based on the interaction between the ionic charge and a flipping induced dipole of a Rydberg atom with a bond length of several micrometers. We measure the vibrational spectrum and spatially resolve the bond length and the angular alignment of the molecule using a high-resolution ion microscope. As a consequence of the large bond length, the molecular dynamics is slow and can be directly observed under the microscope. These results pave the way for future studies of spatio-temporal effects in molecular dynamics, e.g., beyond Born-Oppenheimer physics, and more generally on (ionic) impurities in quantum gases.

Plenary 4: Tuesday, 14:00 - 15:00

The Secret Life of Catalysts: Operando Spectroscopy and Microscopy as Powerful Tools for Mechanistic Understanding

Beatriz Roldán Cuenya

Department of Interface Science, Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Climate change concerns have spurred a growing interest in developing environmentally friendly technologies for green energy generation and storage in the form of chemical bonds. The latter includes green H_2 production from water splitting and the re-utilization of CO_2 via its thermal or electrocatalytic reduction into value-added chemicals and fuels. Moreover, alternative methods for ammonia synthesis either with green H_2 or direct electrocatalytic NH_3 synthesis are also being sought in order to reduce carbon emissions, while providing a transport energy carrier for green hydrogen. In this context, it is thus important to develop low cost, highly efficient and durable catalysts with tunable selectivity. This requires understanding the evolution of their structure and surface/bulk composition under reaction conditions, i.e. while the active sites are formed or become poisoned leading to their deactivation.

This talk will offer new mechanistic insights into the thermal and electrocatalytic reduction of CO_2 and nitrate reduction as well as the oxygen evolution reaction using model pre-catalysts ranging from single atoms to clusters and size- and shape-controlled nanoparticles. I will illustrate the need of a multi-technique operando microscopy and spectroscopy approach, when possible combined, to gain understanding into the complex evolution of catalytic materials while at work. Examples will be given on the correlation between their dynamically evolving structure and composition and their activity and selectivity. These results are expected to open up new routes for the reutilization of CO_2 through its direct conversion into industrially valuable chemicals and fuels such as ethylene, methanol and ethanol, and the generation of green H_2 and ammonia via electrolysis.

Plenary 5: Wednesday, 9:00 - 10:00

Tests of fundamental symmetries using antihydrogen: the ALPHA experiment at CERN

Jeffrey Hangst

Department of Physics and Astronomy, Aarhus University, Denmark

The ALPHA experiment at CERN is unique in its demonstrated ability to study the physical properties of antihydrogen –the antimatter equivalent of the simplest atom. Such studies are motivated by the apparent absence of antimatter in the observable universe, and they probe the fundamental symmetries that underlie current theory. For example, the Standard Model requires that hydrogen and antihydrogen have the same spectrum. The possibility of applying the precision measurement and manipulation techniques of atomic physics to an antimatter atom makes antihydrogen a very compelling testbed for symmetries such as CPT and the Weak Equivalence Principle of General Relativity. To study antihydrogen, it must first be produced, trapped, and then held for long enough to make a measurement –typically using very few anti-atoms. I will discuss the latest developments in antihydrogen physics, including the state-of-the-art of spectroscopic and gravitational studies using the ALPHA-2 and ALPHA-g machines. ALPHA-g is designed to measure the direction and magnitude of the gravitational acceleration of antimatter in the field of the Earth [1]. In ALPHA-2, we have studied several laser and microwave driven transitions and demonstrated laser cooling of trapped antihydrogen [2]. Very recently, we have shown

that it is possible to accumulate more than 104 anti-atoms in a single day. I will illustrate the techniques necessary to achieve these many milestones and consider the future of antihydrogen studies.

[1] Observation of the effect of gravity on the motion of antimatter (ALPHA Collaboration) *Nature* 621,716–722 (2023).

[2] Laser cooling of antihydrogen atoms (ALPHA Collaboration) *Nature* 592, 35–42 (2021).

Plenary 6: Wednesday, 10:30 - 11:30

Negative Ions - Fragile Quantum Systems

Dag Hanstorp

Department of Physics, University of Gothenburg, Sweden

Negative ions, which are formed when electrons are attached to neutral atomic and molecular systems, are unique quantum systems. The lack of a long-range Coulomb force results in the inter-electronic interaction becoming relatively more important. As a consequence, the independent particle model, that adequately describes atomic structure under normal conditions, breaks down. Experimental studies of negative ions can therefore serve to probe correlated electron motion and test theoretical models that go beyond the independent particle approximation.

I will present an overview of experimental methods used to study negative ions, including some recent highlights. The focus will be on the photodetachment process, where one or more electrons are removed from negative ions following the absorption of photons. The experimental results will be compared with state-of-the-art many-body calculations. I will also discuss how the relative simplicity of the structure of negative ions can be used to investigate various fundamental atomic and molecular processes.

Finally, I will discuss the importance of negative ions in various natural environments, such as the interstellar media, and discuss applications of negative ions, where heating of fusion plasmas and trace element analysis will be given as examples.

Plenary 7: Thursday, 9:00 - 10:00

Lighting a path for quantum metrology and fundamental physics

Jun Ye

JILA/National Institute of Standards and Technology, University of Colorado, Boulder, USA

Lasers have fueled revolutionary developments in atomic, molecular, and fundamental physics. Precise optical phase control and quantum technology provide minute-long coherence time for tens of thousands of atoms, enabling the achievement of best measurement precision and accuracy. Ultrafast optics extend coherent light into new spectral regions for observation of novel molecular properties and for precision metrology based on quantum-state-resolved nuclear transition. The permeation of quantum metrology to all corners of physics sparks new ideas for testing fundamental laws of nature and searching for new physics.

Plenary 8: Thursday, 14:00 - 15:00

Dynamics in Atomic and Molecular Physics in the x-ray domain

Marc Simon

Le Laboratoire de Chimie Physique-Matière et Rayonnement, Sorbonne Université, Paris, France

Our research group is working on ultrafast dynamics on isolated atoms and molecules in the x-ray domain using Synchrotron or XFEL. We take advantage of the very short lifetime of core excited species, the creation of multiply charged ions by cascade Auger, emission of fast Auger or x-ray photon of high energy.

We have developed experimental setups allowing to measure x-ray emission, photoemission as well as vectorial coincidences between electrons and ions. We are developing a high-resolution Time-Resolved photoemission setup.

I will show recent results related to the dynamics and spectroscopy of Double Core Hole states [1-4], ultrafast fragmentation examples [5-7] and examples of High photon energy photoionization leading to strong recoil effects [8-10]. Thanks to the fragmentation of multiply charged ions, the localization of inner shells of the CS₂ molecule has been studied [11]. Two examples of attosecond electronic relaxation will be presented [12, 13].

During the talk, I will underline some perspectives of this energy domain in gas phase, with liquids and clusters and on molecules of biological interest.

References

- [1] R. Püttner et al., *Physical Review Letters* **114** 093001 (2015)
- [2] G. Goldsztejn et al. *Physical Review Letters* **117** 133001 (2016)
- [3] T. Marchenko et al., *Physical Review Letters* **119** 133001 (2017)
- [4] I. Ismail et al. *Physical Review Letters* **131** 253201 (2023)
- [5] O. Travnikova et al., *Physical Review Letters* **116** 213001 (2016)
- [6] O. Travnikova et al., *Physical Review Letters* **118** 213001 (2017)
- [7] O. Travnikova et al., *Physical Review Letters* **134** 063003(2025)
- [8] M. Simon et al., *Nature Communications* **5** 4069 (2014)
- [9] E. Kukk et al., *Physical Review Letters* **121** 073002 (2018)
- [10] D. Céolin et al., *PNAS* **116** 4877 (2019)
- [11] R. Guillemin et al., *Nature Communications* **6** 6166 (2015)
- [12] T. Marchenko et al, *Physical Review X* **5** 031021 (2015)
- [13] M. N. Piancastelli et al, *Phys. Rev A* **95** 061402(R) (2017)

Plenary 9: Friday, 9:00 - 10:00

Shedding Light on Nuclear Spins: Through the looking-glass

Mete Atatüre

Department of Physics, University of Cambridge, United Kingdom

Optically active spins in solids are strong candidates for scalable devices towards quantum networks. Semiconductor quantum dots set the state-of-the-art as single-photon sources with high level tuneability, brightness, and indistinguishability. In parallel, their inherently mesoscopic nature leads to a unique realisation of a tripartite interface between light as information carrier, an electron spin as a proxy qubit, and an isolated nuclear spin ensemble. The ability to control these constituents and their mutual interactions create opportunities to realize an optically controllable ensemble of ~50,000 spins. In this talk, I will present a journey from treating the quantum dot nuclei as an uncontrolled noise source limiting spin coherence to the observation of their collective magnon modes and eventually to their function as a quantum register, all witnessed via a single electron spin driven by light.

Spectroscopy 1

Invited Talk, Monday 10:30-11:00, Saal Brüssel

Statistical Analysis of Raman Spectra of Biofuels: The Case of Myristic Acid Conformers

Tsveta Miteva¹; Hela Friha²; Tinihinane Lidia Hidouche¹; Simon Suc²; Jérôme Palaudoux¹; Muneerah Mogren Al-Mogren³; Émilie-Laure Zins⁴; Majdi Hochlaf⁵

¹ Laboratoire de Chimie Physique - Matière et Rayonnement (LCPMR), UMR 7614, CNRS, Sorbonne Université

² Institut Polytechnique des Sciences Avancées (IPSA)

³ Department of Chemistry, Faculty of Sciences, King Saud University

⁴ MONARIS UMR8233, Sorbonne Université, CNRS

⁵ Université Gustave Eiffel, COSYS/IMSE

Biofuels derived from microalgae provide a sustainable alternative to fossil fuels, yet high production costs remain a significant barrier [1]. Optimizing photobioreactors for biofuel production necessitates a detailed understanding of algal biomass, especially its organic components. Raman spectroscopy is a valuable tool for this analysis [2], however, distinguishing individual molecular conformers in complex mixtures remains challenging. This study employs Raman spectroscopy combined with statistical analysis to differentiate fatty acid conformers, using myristic acid as a model system. Density Functional Theory (DFT) calculations (B3LYP-D3/6-311++G**) with solvent effects (water) were used to simulate Raman spectra, achieving a balance between computational efficiency and accuracy. Statistical techniques enabled the classification of myristic acid conformers into chain, v-shaped, and twisted structures, with distinctive vibrational features identified at $\sim 2900\text{ cm}^{-1}$ (CH_2/CH_3 vibrations) and below 1200 cm^{-1} (backbone motions) [3]. This approach enhances the precision of spectral analysis, offering a robust framework for the rapid identification of fatty acids in algal biomass, with implications for biofuel development.

REFERENCES

- [1] Y. Ye, W. Guo, H. H. Ngo, W. Wei, D. Cheng, X. T. Bui, N. B. Hoang, H. Zhang, *Science of The Total Environment* 935 (2024) 172863, <https://doi.org/10.1016/j.scitotenv.2024.172863>.
- [2] K. Czamara, K. Majzner, M. Z. Pacia, K. Kochan, A. Kaczor, M. Baranska, *Journal of Raman Spectroscopy* 46 (1) (2015) 4–20, <https://doi.org/10.1002/jrs.4607>.
- [3] T. Miteva, H. Friha, T. L. Hidouche, S. Suc, J. Palaudoux, M. Mogren Al-Mogren, E. Laure-Zins, M. Hochlaf, *Spectrochimica Acta A* (2025), accepted.

Invited Talk, Monday 11:00-11:30, Saal Brüssel

Molecular conformations in floppy chiral systems probed by Photoelectron Circular Dichroism (PECD)

Laurent Nahon

Synchrotron SOLEIL

Chirality plays a fundamental role in molecular recognition processes. Molecular flexibility is also crucial in molecular recognition, allowing the interacting molecules to adjust their structures and hence optimize

the interaction. Methods probing simultaneously chirality and molecular conformation are therefore crucially needed.

This is the case of a recently-introduced chiroptical effect called Photoelectron Circular Dichroism (PECD) leading to very intense (up to 40 %) forward/backward asymmetries, with respect to the photon axis, in the angular distribution of photoelectrons produced by circularly-polarized light ionization of gas phase pure enantiomers. PECD happens to be an orbital-specific, photon energy dependent chiroptical effect and is a subtle probe of the molecular potential, being very sensitive to static molecular structures such as conformers, isomers, clusters, as well as to vibrational motion, much more so than other observables in photoionization such as the cross section (Photoelectron Spectrum-PES) or the usual (achiral) σ asymmetry parameter (for reviews see [1] [2]).

After an introduction to PECD, several results regarding valence-shell PECD on various floppy systems will be presented, belonging to several cases:

- No control on the conformation distribution, so that only a Boltzmann-averaged global PECD response can be measured, as in the case of the amino-acid alanine.[3,4].
- Partial control : case for which owing to a large binding energy difference between two types of conformers, we could observed directly and rationalize with the help of theoretical calculation a conformer-specific PECD as in the case of amino-acid Proline [5], or for which by changing the carrier gas of the molecular beam it was possible to control the conformer distribution [6], as it is the case of 1-Indanol
- Full conformer selection by using a two-photon ns-laser REMPI scheme as we could demonstrate on 1-indanol [7]

Such a sensitivity to conformation is both an asset and a challenge for the ongoing developments of laser-based PECD techniques as a sensitive chiral (bio)chemical analytical tool in the gas phase.

[1] L. Nahon, G. A. Garcia, and I. Powis, *J. Elec. Spectro. Relat. Phen.* 204, 322 (2015).

[2] R. Hadidi, D. Bozanic, G. Garcia, and L. Nahon, *Adv. Physics: X* 3, 1477530 (2018).

[3] M. Tia, B. Cunha de Miranda, S. Daly, F. Gaie-Levrel, G. Garcia, I. Powis, and L. Nahon, *J. Phys. Chem. Lett.* 4, 2698 (2013).

[4] M. Tia, B. Cunha de Miranda, S. Daly, F. Gaie-Levrel, G. A. Garcia, L. Nahon, and I. Powis, *J. Phys. Chem. A* 118, 2765 (2014).

[5] R. Hadidi, D. K. Božanić, H. Ganjtabar, G. A. Garcia, I. Powis, and L. Nahon, *Commun. Chem.* 4, 72 (2021).

[6] J. Dupont, V. Lepere, A. Zehnacker, S. Hartweg, G. A. Garcia, and L. Nahon, *J. Phys. Chem. Lett.* 13, 2313 (2022).

[7] E. Rouquet, J. Dupont, V. Lepere, G. A. Garcia, L. Nahon, and A. Zehnacker, *Angew. Chem. Int. Ed. Engl.*, e202401423 (2024).

Invited Talk, Monday 11:30-12:00, Saal Brüssel

Towards trapping cold hydrogen molecules

Piotr Wcisło

Nicolaus Copernicus University

Due to its simplicity, H_2 constitutes a perfect tool for testing fundamental physics: testing quantum electrodynamics, determining fundamental constants, or searching for new physics beyond the Standard Model. H_2 has a huge advantage over the other simple calculable systems of having a set of a few hundred ultralong living rovibrational states, which implies the ultimate limit for testing fundamental physics with H_2 at a relative accuracy level of 10^{-24} . The present experiments are far from this limit. I will present our so far results of an ongoing projects aimed at spectroscopy of cold H_2 and trapping cold H_2 . We develop an ultra-strong optical dipole trap. The time-dependent potential is going to recapture the coldest fraction of the cryogenic H_2 cloud.

[1] H Józwiak, P Wcisło, *Scientific Reports* 12, 14529 (2022)

[2] H Józwiak, TV Tscherbul, P Wcisło, *J. Chem. Phys.* 160, 094304 (2024)

[3] K Stankiewicz, et al. <https://arxiv.org/abs/2502.12703>

Hot Topic Talk, Monday 12:00-12:20, Saal Brüssel

Liquid-jet Velocity Map Imaging

Qi Zhou¹; Dominik Stemer¹; Florian Trinter¹; Henrik Haak¹; Uwe Hergenhahn¹; Gerard Meijer¹; Bernd Winter¹; Iain Wilkinson²

¹ Fritz-Haber Institute

² Helmholtz-Zentrum Berlin

Liquid-Jet Photoelectron Spectroscopy (LJ-PES) [1] enables the direct study of the electronic structure of both solute and solvent, and has advanced the chemical analysis in aqueous solutions. The LJ facilitates in-vacuo continuous liquid replacement, and detection of photoelectrons with minimal collisions with evaporating water molecules.

Velocity Map Imaging (VMI) [2] provides optimal photoelectron collection efficiency with a full 4π steradian range, enabling the measurement of photoelectron angular distributions (PADs) in a single image. While VMI is heavily applied to both solid and gaseous phases [3], its intriguing extension to the aqueous phase remains very challenging. Major experimental and technical difficulties include the disturbance of the focusing electric fields by the presence of the dielectric liquid jet, the background resulting from scattering of the photoelectrons with the (aqueous) solution vapor, and the balance between required high electric fields in a high-vapor environment.

We have overcome the most critical technical issues, and have successfully employed our newly developed Liquid-Jet Velocity Map Imaging (LJ-VMI) setup, comprising precisely tunable high-voltage electrodes and a microchannel plate detector. This system offers a broad dynamical energy range, allowing detection of photoelectrons kinetic energies up to approximately 40 eV. Following initial lab-experiments using laser and ultraviolet light sources, we present here our recent LJ-VMI results obtained at the bending-magnet beamline PM3, at the BESSY-II synchrotron-radiation facility. Data are presented for water, aqueous solutions, as well as non-aqueous solution. We report solute and solvent core-level and valence electron binding energies, show associated PADs, and identify the principal effects of a liquid jet in VMI performance. Next steps in our continuous development of LJ-VMI will be discussed, along the perspective for future applications towards near-ionization-threshold phenomena as well as time-resolved photo-induced reactions and electron dynamics in (aqueous) solution.

[1] B. Winter, M. Faubel, Chem. Rev., 106, 4, pp. 1176–1211, (2006)

[2] A. Eppink, D. Parker, Rev. Sci. Instrum., 68(9), pp. 3477–3484, (1997)

[3] D. M. Neumark, J. Phys. Chem. A, 127, 4207–4223, (2023)

Hot Topic Talk, Monday 12:20-12:40, Saal Brüssel

Core-level electron transfer mediated decay in microhydrated pyrimidine

Madhusree Roy Chowdhury¹; Lassi Pihlava²; Marta Berhotlz³; Edwin Kukk²; Arno Ehresmann¹; Andreas Hans¹

¹ University of Kassel

² University of Turku

³ University of Tartu

The absorption of soft X-ray photons by biological matter can lead to core-level ionization, producing excited cation radicals with the deposition of large amount of energy. The excited molecule relaxes by different competing relaxation channels, emitting a photon or release of a secondary electron called Auger electron where the core-level vacancy is filled by an outer-valence electron and the excess energy is

used to emit another outer-valence electron from the same molecule. The doubly charged molecule mostly undergoes fragmentation. If the biomolecule is embedded in an environment, then apart from the local decay channels there can be different non-local decay processes involving both the biomolecule and its neighbours. One such non-local decay channel is the intermolecular Coulombic decay (ICD) [1] where the energy released from the relaxation of the initially core ionized molecule is transferred to a neighboring molecule that uses it to emit one of its electrons. Another decay channel is the electron-transfer mediated decay (ETMD) [2] where the core vacancy of the initially ionized molecule is filled by an electron from the neighboring molecule and another electron is emitted from yet another neighbor. Thus two vacancies are formed on two neighbors while the initially ionized molecule becomes neutral. These nonlocal decay mechanisms have mostly been considered to have minor contribution in case of inner-shell (core-level) vacancies, accounting for a few percent compared to the predominant Auger decay channel. However, a recent study showed experimentally that core-level ICD is an important channel for X-ray induced core-level ionization of microsolvated pyrimidine molecules [3] and theoretical calculations revealed a high branching ratio of non-local channels along with predicting a significant intensity for core-level ETMD channel. In the context of radiation damage to biological matter, such local and non-local competing decay channels can produce several low energy secondary electrons and water radicals which are the key players for causing single and/or double strand breaks in the DNA/RNA of the cells.

In the present work, we study the X-ray photoionization and fragmentation of pyrimidine embedded in water cluster to experimentally verify the core-level ETMD channel using the photoelectron-photoion-photoion coincidence (PEPIPICO) spectrometer connected at the gas phase endstation of the Finnish-Estonian beamline (FinEstBeAMS) [4] at the MAX IV synchrotron radiation facility. The PEPIPICO coincidence maps measured in coincidence with the C 1s photoelectron of pyrimidine shows signature of non-local processes especially the ETMD channel causing ionization of the neighboring water molecules to distribute the internal energy to the environment when the pyrimidine is ionized by the initial irradiation.

References

[1] T. Jahnke *et al.*, Chem. Rev. **120**, 11295 (2020)

[2] M. Förstel *et al.*, Phys. Rev. Lett. **106**, 033402 (2011)

[3] A. Hans *et al.*, J Phys. Chem. Lett. **12**, 7146 (2021)

[4] K. Kooser *et al.*, J. Synchrotron Rad., **27**, 1080 (2020)

Ultrafast 1

Invited Talk, Monday 10:30-11:00, Saal Tirol

Ultrafast preparation and detection of entangled atoms using a COLTRIMS reaction microscope

Sebastian Eckart

Goethe-Universität Frankfurt

We report on experiments with highly intense femtosecond laser pulses with tailored polarization to study entanglement of spatially separated atoms on femtosecond time scales.

Previously, it has been shown that circularly polarized light favors electrons with a certain magnetic quantum number in strong field ionization [1]. This preference was used to prepare and detect ring currents in single argon ions [2,3].

Building on these insights, we use a pump-probe scheme to prepare and detect ring currents in dissociating oxygen molecules. The laser pulses have intensities on the order of 10^{14} W/cm².

The pump pulse excites a ring current in molecular oxygen and simultaneously triggers the dissociation of the molecule into two spatially separated entangled oxygen atoms. The probe pulse allows us to investigate this pair of atoms on femtosecond time scales. We find that the valence electrons of the two atoms are entangled in their magnetic quantum number [5].

The momenta of the liberated electrons and the ions are measured in coincidence using cold-target recoil-ion momentum spectroscopy (COLTRIMS) reaction microscopes [4].

- [1] I. Barth, O. Smirnova, *Phys. Rev. A* **84**, 063415, (2012)
- [2] T. Herath et al., *Phys. Rev. Lett.* **109**, 043004, (2012)
- [3] S. Eckart et al., *Nat. Phys.* **14**, 701, (2018)
- [4] J. Ullrich et al., *Rep. Prog. Phys.* **66**, 1463, (2003)
- [5] S. Eckart et al., *Science Advances* **9**, eabq8227, (2023)

Invited Talk, Monday 11:00-11:30, Saal Tirol

X-ray superfluorescence

Nina Rohringer

DESY, Hamburg

X-ray free-electron lasers (XFELs) open new avenues towards studying collective x-ray emission and nonlinear x-ray matter interaction. In this talk I will present recent advancements on the experimental and theoretical exploration of collective spontaneous x-ray emission (x-ray superfluorescence) following ultrafast inner-shell photoionization. X-ray superfluorescence has been demonstrated in atomic gases in the soft x-ray range [1], in rare-gases [2] and clusters [3] in the XUV, and in solids and liquids in the hard x-ray range [4,5]. As opposed to the XFEL pulses that are based on the process of self-amplified spontaneous emission and have limited temporal coherence, x-ray superfluorescence produces phase-stable, ultrabright x-ray pulses of fs and sub-fs duration [6,7]. A quantitative theoretical prediction of this effect is intricate and computationally demanding, since it involves incoherent pumping of a large ensemble of atoms of several electronic states that undergo strong decoherence through electronic decay channels and pulse propagation effects, along with the need of a quantum-electrodynamical description of the field modes. I will present a theoretical framework [8,9] strongly linked to stochastic sampling of the time-dependent positive-P distribution of the multi-dimensional Liouville space. In this novel method, we extend a previous phenomenological treatment and treat quantum fluctuations of the electromagnetic field by appropriate stochastic contributions. The resulting set of coupled stochastic partial differential equations resemble the generalized Maxwell-Bloch equations to follow the evolution of the electromagnetic fields and the density matrix of the emitters [10]. The stability of the equations will be discussed and I address potential applications of the method in cavity and nonlinear quantum optics.

- [1] N. Rohringer et al., *Nature* **481**, 488 (2012).
- [2] L. Mercadier et al., *Physical Review Letters* **123**, 023201 (2019).
- [3] A. Benediktovitch et al. *Physical Review A* **101**, 063412 (2020).
- [4] T. Kroll et al., *Physical Review Letters* **120**, 133203 (2018).
- [5] T. Kroll et al., *Physical Review Letters* **125** (3), 037404 (2020).
- [6] M. D. Doyle et al., *Optica* **10**, 1602 (2023).
- [7] T. M. Linker et al., *Nature*, accepted (2025). <https://arxiv.org/abs/2409.06914>
- [8] S. Chuchurka, V. Sukharnikov, A. Benediktovitch and N. Rohringer, *Phys. Rev. A* **110**, 053703 (2024).
- [9] S. Chuchurka, V. Sukharnikov and N. Rohringer, *Phys. Rev. A* **109**, 063705 (2024).
- [10] S. Chuchurka, A. Benediktovitch, Š. Krušič, A. Halavanau, and N. Rohringer, *Phys. Rev. A* **109**, 03375 (2024).

Invited Talk, Monday 11:30-12:00, Saal Tirol

Shaping light in 3D to twist electrons on an ultrafast timescale

David Ayuso

Imperial College London

Chirality—the property of an object that cannot be superimposed on its mirror image—is ubiquitous in nature. Like our hands, opposite versions of the same chiral molecule (R and S enantiomers) behave identically unless they interact with another chiral object. Molecular chirality is rapidly becoming essential in nanotechnology [1], e.g. for developing molecular motors and spintronic devices. The unbalance between R and S biomolecules on Earth (amino acids, sugars, DNA, etc.) supports life. This homochirality gives different biological activities to opposite versions of a chiral drug or pesticide, with profound implications for pharmaceuticals and agriculture. Moreover, abnormal enantiomeric ratios of chiral biomarkers have recently been linked to cancer, Alzheimer's, diabetes, and other diseases [2].

Having efficient tools for rapid chiral discrimination is therefore vital. However, current optical methods are inefficient because they rely on the (chiral) helix that circularly polarised light draws in *space*. The pitch of this helix—determined by light's wavelength—is ~10,000 times larger than the molecules. Consequently, the molecules perceive the helix as a flat circle, hardly feeling its chirality. This results in weak chiral sensitivity, typically <0.1%, which presents major limitations [3]. We can overcome these limitations by creating synthetic chiral light [4-6], where the tip of the electric-field vector traces a 3D chiral trajectory in *time*. This new type of chiral light can drive ultrafast chiral currents inside the molecules, which interact with the chiral molecular skeleton in a highly enantiosensitive manner, leading to 100% chiral sensitivity.

In this presentation, I will show how we can shape light's polarisation in 3D to achieve highly efficient chiral sensing [4-10] and manipulation [11], together with theoretical and computational results that support the feasibility of our approaches. Current optical instrumentation enables several strategies for 3D shaping, such as using several laser beams that propagate non-collinearly [4-6,11], only one beam but tightly focused [7,8], vortex beams to create topological chiral light [9], or ultrafast TACOS [10]. I will discuss how these ideas enable highly efficient chiroptical sensing via high harmonic generation using strong fields, as well as gentle chiroptical imaging in the low-order perturbative regime.

- [1] J. Brandt et al, *Nature Reviews Chemistry* **1**, 0045 (2017)
- [2] Y. Liu et al, *Nature Reviews Chemistry* **7**, 355 (2023)
- [3] D. Ayuso et al, *Phys Chem Chem Phys* **24**, 26962 (2022)
- [4] D. Ayuso et al, *Nature Photonics* **13**, 866 (2019)
- [5] D. Ayuso et al, *Nature Communications* **12**, 3951 (2021)
- [6] J. Vogwell et al, *Science Advances* **9**, eadj1429 (2023)
- [7] D. Ayuso et al, *Optica* **8**, 1243 (2021)
- [8] L. Rego et al, *Nanophotonics* **12**, 14, 2873 (2023)
- [9] N. Mayer et al, *Nature Photonics* **18**, 1155 (2024)
- [10] J. Terentjevas et al, *ArXiv:2406.14258v1* (2024)
- [11] A. Ordóñez et al, *ArXiv:2309.02392* (2023)

Hot Topic Talk, Monday 12:00-12:20, Saal Tirol

Measurement and control of interactions in bosonic optical clocks

Marco Tarallo

INRIM

We report precise measurements of inter-species interactions in a

bosonic optical lattice clock based on ^{88}Sr atoms [1]. We observe a nonlinear behavior of the clock density shift, showing features deriving from many-body physics beyond the mean-field theory, even without reaching the quantum degeneracy. This findings enable a cancellation of the density shift systematic effect through a careful choice of a “magic” density and excitation fraction. We discuss the implications of these findings in many-body physics, quantum simulation [2], and precision isotope shift measurements [3], which provide a powerful probe for new physics beyond the Standard Model [4].

[1] J.P. Salvatierra, et al, in preparation (2025).

[2] T. Comparin, et al., Phys. Rev. Lett. 129, 113201 (2022)

[3] H. Miyake, et al., Phys. Rev. Research 1, 033113 (2019)

[4] J. Berengut, et al., Phys. Rev. Lett. 120, 091801 (2018)

Hot Topic Talk, Monday 12:20-12:40, Saal Tirol

Entanglement-Enhanced Atomic Gravimeter

Christophe Cassens¹; Bernd Meyer-Hoppe¹; Ernst Rasel²; Carsten Klempt¹

¹ Deutsches Zentrum für Luft- und Raumfahrt SI; Institut für Quantenoptik, Leibniz Universität Hannover

² Leibniz Universität Hannover, Institut für Quantenoptik

Interferometers based on ultracold atoms enable an absolute measurement of inertial forces with unprecedented precision. However, their resolution is fundamentally restricted by quantum fluctuations. Improved resolutions with entangled or squeezed atoms were demonstrated in internal-state measurements for thermal and quantum-degenerate atoms and, recently, for momentum-state interferometers with laser-cooled atoms. Here, we present a gravimeter based on Bose-Einstein condensates with a sensitivity of $-1.7_{-0.5}^{+0.4}$ dB beyond the standard quantum limit. Interferometry with Bose-Einstein condensates combined with delta-kick collimation minimizes atom loss in and improves scalability of the interferometer to very-long-baseline atom interferometers.

Collisions 1

Invited Talk, Monday 17:00-17:30, Saal Tirol

Controlled collisions of molecules and ions

Stefan Willitsch

University of Basel

Recent advances in the control of the energy, quantum state and even shape of neutral molecules and molecular ions in the gas phase have opened up new possibilities for detailed studies of molecular interactions, collisions and chemical reactions. In the talk, we will present a range of recent results and new experimental developments which are all joined by the common theme of using controlled molecules for studies of collisional and chemical dynamics. First, we will discuss experimental techniques for the preparation of individual conformations of both neutral molecules and molecular ions and their use in the investigation of conformational effects in chemi-ionisation and ion-molecule reactions. Second, we will highlight how recently developed quantum-logic assisted protocols for molecular state readout can be employed for exploring the state-to-state dynamics of molecular collisions with high sensitivity on the single-molecule level. Third, we will present

a new approach for the simultaneous (“hybrid”) trapping of cold neutral molecules and ions for studies of ion-molecule processes in the millikelvin regime. The talk will conclude with an outlook on future developments.

Invited Talk, Monday 17:30-18:00, Saal Tirol

Reactive collisions of oxygen atoms with aromatic compounds in crossed-beam experiments

Nadia Balucani

University Of Perugia

In our laboratory, we have started a systematic investigation of the reactions involving oxygen atoms and aromatic compounds under single collision conditions using the crossed molecular beam technique with mass spectrometric detection. The first systems we have looked at are $\text{O}(\text{^3P}) + \text{benzene}$ [1], pyridine [2], and toluene [3]. More recent results are on $\text{O}(\text{^3P}) + \text{ethylbenzene}$ and $\text{O}(\text{^3P}) + \text{thiophene}$, while we plan to investigate the reactions with styrene, anisole, and other functionalized aromatics.

A detailed understanding of these reactive systems has practical implications ranging from biomass gasification to the design of novel space-technology aromatic polymers resistant to the attack by the oxygen atoms in the Low Earth Orbit, where most satellites reside. From a fundamental point of view, these studies aim to derive the structure dependency of the reactivity of aromatics.

As in the case of the $\text{O}(\text{^3P})$ reactions with unsaturated organic compounds, the investigated reactions are strongly affected by intersystem crossing (ISC) to the underlying singlet potential energy surface with a significant alteration of the reaction mechanism and product branching fractions. ISC can occur in the entrance channel, as observed for the $\text{O} + \text{pyridine}$ reaction [2], or at a later stage. In all cases, upon ISC, either ring-contraction or ring-opening (in the case of $\text{O} + \text{thiophene}$) mechanisms with CO-elimination were observed to be significant or dominant (in the case of the reaction with pyridine and thiophene). The experimental results are interpreted with the help of ad hoc theoretical simulations.

[1] G. Vanuzzo et al., J. Phys. Chem. A **125**, 8434 (2021)

[2] P. Recio et al., Nature Chemistry **14**, 1405 (2022)

[3] N. Balucani et al., Faraday Disc. **251**, 523 (2024)

We acknowledge financial support under the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 104 published on 02.02.2022 by the Italian Ministry of University and Research (MUR), funded by the European Union – NextGenerationEU – Project Title 20227W5CLJ Biomass gasification for hydrogen production (Bio4H2) – CUP J53D23001970006 - Grant Assignment Decree No. 961 adopted on 30.06.2023 by the Italian Ministry of Ministry of University and Research (MUR).

Hot Topic Talk, Monday 18:00-18:20, Saal Tirol

The Mutual Neutralization of Hydronium and Hydroxide.

Alon Bogot¹; Arnaud Dochain²; Daniel Strasser¹;
Henning Schmidt²; Henning Zettergren²; Mathias
Poline²; MingChao Ji²; Richard Thomas²

¹ Hebrew university of Jerusalem

² Stockholm University

The feasibility of performing merged beam experiments with trapped fast ion beams of molecular cations and anions at the double electrostatic storage ring (DESIREE) and the hybrid electrostatic ion beam trap (HEIBT), [1,2] opens new opportunities to study mutual neutralization reactions. Here, I will present our findings from merged beam experiments performed at DESIREE on the mutual neutralization of hydronium (H₃O⁺) and hydroxide (OH⁻), [3] and their isotopomers. [4] 3D coincidence imaging of the neutral products allowed us to disentangle the different competing proton-transfer and electron-transfer mechanisms. We identified a predominant e-transfer mechanism that forms either one or two OH radicals in a single neutralization reaction. By analyzing measured 3-body momentum correlations, we found that the distance at which the electron transfer occurs determines the final product channel. Electron transfer at a distance of ~4 Å forms the neutral H₃O radical intermediate ground state, which then dissociates into H₂O and H. In contrast, electron transfer at ~10 Å forms an electronically excited H₃O intermediate that dissociates into H₂ and a 2nd OH radical. These mutual neutralization dynamics of the isolated water ions can be related to ion-ion reactions on the liquid water surface and offer an explanation for the recent observations of spontaneous hydrogen peroxide formation in pure water microdroplets. [5-7]

References

- [1] A. Bogot et al, Phys. Chem. Chem. Phys., 25, 25701-25710 (2023)
- [2] H.T. Schmidt et al, Rev. Sci. Instrum., 84, 055115 (2013)
- [3] A. Bogot et al, Science, 383, 285-289 (2024)
- [4] A. Bogot et al, preprint available at Research Square <https://doi.org/10.21203/rs.3.rs-4777257/v1>
- [5] J.K. Lee et al, PNAS, 116 (39), 19294-19298 (2019)
- [6] P. Skurski and J. Simons, J. Chem. Phys., 160, 034708 (2024)
- [7] J.P. Heindel et al, Nat Commun, 15, 3670 (2024)

Hot Topic Talk, Monday 18:20-18:40, Saal Tirol

Quantum State Selection and Laser Cooling Systems for Studying Collisions and Reaction Dynamics at Low Temperatures

Tiangang Yang

Southern University of Science and Technology (SUSTech)

Quantum state-selected scattering at low temperatures is essential for understanding molecular reaction dynamics and the chemistry of astrophysical processes. A key aspect of these studies is the use of techniques that cool reactants and precisely select their quantum states. We have recently enhanced our research capabilities by integrating a laser-cooled ion trap with a high-resolution time-of-flight mass spectrometer (TOF-MS) and fluorescence imaging. Additionally, we have developed a cooling apparatus for Be⁺ and C⁺ ions that achieves subkelvin temperatures using laser and sympathetic cooling. This setup provides meticulous control over ion micromotion, significantly improving our ability to explore ion-molecule reactions across diverse collision energies. Furthermore, by leveraging ion motional heating, we have achieved two-dimensional cooling of Be⁺ ions without the need for repump laser beams.

Moreover, our setup incorporates a stimulated Raman pumping (SRP) system paired with a fast chopper to achieve high-efficiency molecular state selection for H₂ and N₂. Furthermore, by integrating a cavity-enhanced infrared excitation scheme with a milliwatt laser, we achieved over 30% efficiency in exciting the overtone transition of CO (v=3), enabling detailed studies of state-selected reaction dynamics. In this talk, I will discuss recent advancements in this project, as well as ongoing ion-molecule reaction studies utilizing these systems.

Quantum 1

Invited Talk, Monday 17:00-17:30, Saal Brüssel

Rethinking Resonance Fluorescence: Fundamental Insights and Emerging Quantum Technologies

Arno Rauschenbeutel

Department of Physics, Humboldt-Universität zu Berlin, Germany

Resonance fluorescence—the light emitted by a coherently driven two-level quantum emitter—has long served as a paradigm in quantum optics. In this talk, I will present two recent experimental investigations that reveal both the fundamental richness and the technological potential of this seemingly simple system (1,2). In the first part, I revisit the textbook notion that a single atom cannot scatter two photons simultaneously. Our results provide direct experimental evidence for an alternative quantum interference-based explanation, in which antibunching emerges from the coherent superposition of distinct two-photon scattering amplitudes. By selectively suppressing the coherently scattered component of the fluorescence spectrum, we isolate photon pairs that are simultaneously scattered by the atom, thereby validating a decades-old theoretical prediction. In the second part, I will show how resonance fluorescence can be harnessed as a highly efficient source of time-bin entangled photon pairs. Using beam splitters, delay lines, and post-selection only, we transform the emission from a single atom into a stream of maximally entangled photon pairs, achieving a strong violation of a Bell inequality. Together, these experiments illustrate how resonance fluorescence—traditionally viewed as a fundamental textbook example—can be reimagined as a powerful resource for quantum information science.

1. L. Masters *et al.*, *Nature Photonics* **17**, 972 (2023)

2. X.-X. Hu *et al.*, *arXiv:2504.11294*

Hot Topic Talk, Monday 18:00-18:20, Saal Brüssel

Protecting collective qubits

Antoine Covolo; Valentin Magro; Mathieu Girard;
Sebastien Garcia; Alexei Ourjoumtsev

JEIP, UAR 3573 CNRS, Collège de France, PSL University

Collective atomic or solid-state excitations present important advantages for encoding qubits, such as strong directional coupling to light. Unfortunately, they are plagued by inhomogeneities between the emitters, which make the qubit decay into a quasi-continuum of dark states. In most cases, this process is non-Markovian. Through a simple and resource-efficient formalism, we unveil a regime where the decay is suppressed by a combination of driving and non-Markovianity. We experimentally demonstrate this “driving protection” using a Rydberg

superatom, extending its coherent dynamics beyond the characteristic free decay time by an order of magnitude [1].

[1] A. Covolo et al, arXiv:2501.07232.

Hot Topic Talk, Monday 18:20-18:40, Saal Brüssel

Observation of anomalous information scrambling in a Rydberg atom array

Xinhui Liang¹; Zonpei Yue¹; Yuxin Chao¹; Zhenxing Hua¹; Yige Lin²; Meng Khoon Tey¹; Li You¹

¹ Tsinghua University

² National Institute of Metrology of China

Study of information scrambling in a quantum many-body system is key to understanding the dynamics of thermalization and the evolution towards equilibrium. This work reports our experimental investigation into this topical subject by directly observing the out-of-time-order correlation (OTOC) function in a Rydberg atom array.

A key challenge in measuring the OTOC in an analog-digital hybrid circuit is the difficulty of implementing time-reversed evolution. We address this by leveraging the inherent constraints imposed by the strong van der Waals interactions in the Rydberg atom array system.

Our observations show that the scrambling dynamics for quantum many-body scar in a Rydberg atom array is anomalous, accompanied by a linear lightcone with a smaller valued butterfly velocity and persistent periodic oscillations inside, which differs from both thermal and many-body localized systems, and signifies an unusual breakdown of thermalization.

If time permits, I will briefly mention our another experiment on disorder-induced topology in a Rydberg atom array.

Large Systems 1

Invited Talk, Tuesday 10:30-11:00, Saal Straßburg

Exploring quantum Hall physics with ultracold dysprosium atoms

Sylvain Nascimbene

CNRS - Laboratoire Kastler Brossel

Ultracold atomic gases offer a versatile platform for exploring rich phenomena in quantum matter. In particular, topological states akin to those found in the quantum Hall effect can be engineered by simulating orbital magnetic fields—an approach greatly facilitated by the use of synthetic dimensions.

In this talk, I will present our experimental realization of a quantum Hall system using ultracold gases of dysprosium atoms. By leveraging the atom's large internal spin ($J = 8$), we encode a synthetic dimension and couple it to atomic motion via two-photon optical transitions, which generates an effective magnetic field. We observe hallmark signatures of quantum Hall physics, including a quantized Hall response and gapless, chiral edge modes.

I will then describe a more intricate experiment designed to probe spatial entanglement by simulating the so-called entanglement Hamiltonian. Using the Bisognano-Wichmann theorem—which relates the entanglement Hamiltonian to a spatially deformed version of the original system—we implement this deformation along the synthetic dimension.

Lastly, I will discuss our recent investigation into a topological phase transition, induced by introducing an additional lattice potential. I will highlight the system's behavior in the critical regime and explore the emergent features associated with the transition.

Invited Talk, Tuesday 11:00-11:30, Saal Straßburg

Electronic Quantum Dynamics in Helium Droplets traced by Coherent Diffractive Imaging

Thomas Fennel

Uni Rostock

Single-Shot Coherent Diffractive Imaging (CDI) has become a mature tool to capture the structure and dynamics of nanoscale systems such as viruses [1], nanoparticles [2] and helium droplets in free flight [3]. The conventional application of the underlying single-shot imaging implies that the imaging pulse interacts instantly and perturbatively with the target such that the diffraction image reflects the target shape and (unperturbed) optical properties via the linear-response field propagation through (and around) the target. Especially the advancing capabilities of intense XUV light sources render the question important, at which point non-linear quantum state dynamics driven by the imaging pulse become significant [4]. In this talk I will discuss an attempt to tackle this question theoretically by means of scattering simulations that include field propagation and local quantum state dynamics for the example of Helium droplets [5]. It will be shown for the example of resonantly driven Helium droplets that the departure from the strictly linear regime may open up a wide range of opportunities to track and drive quantum state population dynamics [6]. Emerging routes for associated new metrologies in the field of CDI will be discussed.

- [1] M. Seibert et al., Nature 470, 78 (2011)
- [2] C. Peltz et al., New J. Phys. 24, 043024 (2022)
- [3] Gomez et al., Science 345, 907 (2014)
- [4] D. Rupp et al., Nat. Commun. 8, 493 (2017)
- [5] B. Kruse et al., J. Phys. Photonics 2, 024007 (2020)
- [6] B. Kruse, PhD thesis, University of Rostock (2024)

Invited Talk, Tuesday 11:30-12:00, Saal Straßburg

Ultrafast relaxation processes in photoexcited He nanodroplets

Marcel Mudrich

Aarhus University

Helium nanodroplets are quantum fluid clusters that feature extraordinary properties such as ultralow temperature and superfluidity. They have mostly been used as inert nanometer-sized cryo-matrices for isolating molecules and for aggregating molecular complexes and nanostructures that are hard or impossible to form by other means. However, when helium nanodroplets are resonantly excited or photoionized, they turn into a highly reactive species that feature a complex reaction dynamics.

In this contribution I'll present experiments probing the ultrafast dynamics of pure and doped helium nanodroplets initiated by resonant photoexcitation and ionization of the helium droplets. Using synchrotron radiation, free-electron lasers and high-harmonic generation sources, we track ultrafast relaxation processes such as internal conversion, bubble formation, as well as energy- and charge-transfer ionization between (super-)excited helium atoms and between helium atoms and attached dopant atoms and molecules [1-5]. In particular, interatomic Coulombic decay (ICD) processes prevail nearly in the entire extreme-ultraviolet range of the spectrum [6-12]. ICD is initiated by resonant single or double excitation [6,7], simultaneous ionization and excitation [8], and indirectly by photoelectron impact excitation [9,10]. By forming tailored complexes in helium nanodroplets, their ionization and fragmentation dynamics can be studied under controlled conditions [12,13].

References

- [1] C. Medina et al., New Journal of Physics 25, 053030 (2023).
- [2] A. C. LaForge et al., PCCP 24, 28844-28852 (2022).
- [3] J. D. Asmussen et al., J. Phys. Chem. Lett. 13, 4470-4478 (2022).
- [4] A. C. LaForge et al., Phys. Rev. X 11, 021011 (2021).
- [5] J. D. Asmussen et al., J. Chem. Phys. 159, 034301 (2023).
- [6] L. Ben Ltaief et al., Phys. Rev. Research 6, 013019 (2024).
- [7] B. Bastian et al., Phys. Rev. Lett. 132, 233001 (2024).
- [8] M. Shcherbinin et al., Phys. Rev. A 96, 013407 (2017).
- [9] L. Ben Ltaief et al., Phys. Rev. Lett. 131, 023001 (2023).
- [10] L. Ben Ltaief et al., Rep. Prog. Phys. 88, 037901 (2025).
- [11] A. C. LaForge et al., Rep. Prog. Phys. 87, 126402 (2024).
- [12] J. D. Asmussen et al., PCCP 25, 24819-24828 (2023).
- [13] S. De et al., J. Chem. Phys. 160, 094308 (2024).

Hot Topic Talk, Tuesday 12:00-12:20, Saal Straßburg

Peptide bonds formation in clusters of amino acids in the gas phase induced by ionizing radiation.

Mariana Leiferman Tamames¹; Michal Roth²; Ori Licht²; Sumit Srivastav³; Fernando Aguilar-Galindo⁴; Yoni Toker²; Patrick Rousseau³; Sergio Díaz-Tendero⁵

¹ Universidad Autónoma de Madrid

² Physics Department and Institute for Nanotechnology and Advanced Materials, Bar-Ilan University

³ Normandie University, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP

⁴ Universidad Autónoma de Madrid, IAdChem

⁵ Universidad Autónoma de Madrid, IAdChem, IFIMAC

In this communication we present how ionizing radiation influences the formation of peptide bonds in clusters of amino acids in the gas phase. In the past, simulations and experiments were carried out in parallel to understand the possible mechanisms involved[1,2]. Due to these promising previous results, we have expanded the study, including clusters of other amino acids. The main objective of this study is to evaluate the conditions of peptide bond formation in pure clusters of glycine, threonine, valine, serine and cysteine in the gas phase induced by collisions with alpha particles.

Experimentally, mass spectrometry is used to analyze the charged species formed after the collision with the highly charged ions. From the theoretical point of view, first the search for conformers is carried out using the CREST program[3], and then the structures obtained are further reoptimized with the Gaussian16 software[4] using the density functional theory DFT. The second stage of the work has been to make an analogous study, but on protonated clusters, since in these species believed to play the key role in the experiments. Finally, we have explored the potential energy surfaces to locate the transition states that explains the mechanism for peptide bond formation from the protonated clusters, also using DFT.

Hot Topic Talk, Tuesday 12:20-12:40, Saal Straßburg

Cryogenic single nanoparticle mass spectrometry

Björn Bastian; Kleopatra Papagrigoriou; Sophia C. Leippe; Knut R. Asmis

Universität Leipzig

Nanoparticle (NP) mass spectrometry in the gas phase is a unique way to characterize individual isolated particles and thus assess their intrinsic properties, NP-to-NP variability and structural evolution, e.g. in studies on charging mechanisms [1], photophysics [2] or high temperature reaction kinetics [3]. Our group focuses on cryogenic experiments to employ absorption spectroscopy, based on adsorption of messenger atoms or molecules on the NP surface and their desorption driven by laser heating with rates that are proportional to the absorption cross section [4]. An overview is given over the related goals, challenges and progress in charge state control, fluorescence thermometry [5] with the aim for temperature controlled experiments, and quantitative characterization of the adsorption on a NP surface.

[1] M. Grimm et al., Phys. Rev. Lett. 96, 066801 (2006)

[2] V. Dryza et al., Phys. Chem. Chem. Phys. 15, 20326 (2013)

[3] C. Y. Lau et al., J. Phys. Chem. C 127 (31), 15157 (2023)

[4] B. Hoffmann et al., J. Phys. Chem. Lett. 11, 6051 (2020)

[5] S. C. Leippe et al., J. Phys. Chem. C 128 (50), 21472 (2024)

Quantum 2

Invited Talk, Tuesday 10:30-11:00, Saal Tirol

Quantum interfaces with ions and nanoparticles

Tracy Eleanor Northup

University of Innsbruck

Coupling a spin qubit to a mechanical system provides a route to prepare the mechanical system's motion in nonclassical states, such as a Fock state or an entangled state. Such quantum states have already been realized with superconducting qubits coupled to clamped mechanical oscillators; here, we are interested in achieving an analogous coupling between an atomic spin and a levitated oscillator, namely, between a trapped calcium ion and a silica nanoparticle in a linear Paul trap. Levitated systems offer extreme isolation from the environment and the possibility to dynamically adjust the oscillator's confining potential, providing a path for the generation of macroscopic quantum superpositions.

I will present recent steps in this direction: First, we have adapted techniques originally developed for trapped atomic ions, including detection via self-interference and sympathetic cooling, for the domain of nanoparticles [1,2]. Second, we have confined a nanoparticle oscillator in ultra-high vacuum and obtained quality factors above 10^{10} , evidence of its extreme isolation from its environment [3]. Finally, we have trapped a calcium ion and a nanoparticle together in a linear Paul trap, taking advantage of a dual-frequency trapping scheme [4].

[1] L. Dania, K. Heidegger, D. S. Bykov, G. Cerchiari, G. Arenada, T. E. Northup, Phys. Rev. Lett. 129, 013601 (2022)

[2] D. S. Bykov, L. Dania, F. Goschin, T. E. Northup, Optica 10, 438 (2023)

[3] L. Dania, D. S. Bykov, F. Goschin, M. Teller, A. Kassid, T. E. Northup, Phys. Rev. Lett. 132, 133602 (2024)

[4] D. Bykov, L. Dania, F. Goschin, T. E. Northup, arXiv:2403.02034 (2024)

Invited Talk, Tuesday 11:00-11:30, Saal Tirol

Non-local quantum many-body systems

Carlos Barahona-Pascual; Hong Jiang; Alan C. Santos; Juan José García Ripoll

Institute of Fundamental Physics, IFF-CSIC

In this talk I will describe our work on quantum networks of quantum emitters [1]. From the point of view of Quantum Optics, these are setups of quantum emitters (i.e. qubits or cavities that talk to qubits) connected by waveguides that transport photons among those nodes. This leads to a paradigm of quantum systems interacting through the exchange of retarded photons, creating what we call a non-local quantum many-body system. I will discuss the theoretical tools we have developed and how these tools can already provide insight in topics ranging from quantum state transfer among quantum processors to a

new type of collective emission, called cascaded superradiance, that takes place in these networks.

[1] *Time-delayed collective dynamics in waveguide QED and bosonic quantum networks*, Carlos Barahona-Pascual, Hong Jiang, Alan C. Santos, Juan José García-Ripoll, [arXiv:2505.02642](https://arxiv.org/abs/2505.02642)

Invited Talk, Tuesday 11:30-12:00, Saal Tirol

Building a quantum network one photon at a time

Rob Thew

University of Geneva

The generation and distribution of entanglement as a resource is one of the big challenges for the field of quantum communication. We discuss some of our work on single photon entanglement and building up complex quantum states from individual photons for use in quantum networks. In particular, some of our recent work looks at going beyond entanglement swapping to heralding entanglement at a distance, which is of relevance for quantum repeaters as well as device-independent QKD. We finish with a quick look at how we're developing photonic sources compatible with quantum memories and some recent results on photon number resolving detectors

Hot Topic Talk, Tuesday 12:00-12:20, Saal Tirol

Self-Assembled Chains and Solids of Dipolar Atoms in a Multilayer

Grecia Guijarro¹; Gregory Astrakharchik¹; Giovanna Morigi²; Jordi Boronat Médico¹

¹ Universitat Politècnica de Catalunya

² Saarland University

We predict that ultracold bosonic dipolar gases, confined within a multilayer geometry, may undergo self-assembling processes, leading to the formation of chain gases and solids. These dipolar chains, with dipoles aligned across different layers, emerge at low densities and resemble phases observed in liquid crystals, such as nematic and smectic phases. We calculate the phase diagram using quantum Monte Carlo methods, introducing a newly devised trial wave function designed for describing the chain gas, where dipoles from different layers form chains without in-plane long-range order. We find gas, solid, and chain phases, along with quantum phase transitions between these states. Specifically, we predict the existence of quantum phase transitions from gaseous to self-ordered phases, as the interlayer distance is decreased. Remarkably, in the self-organized phases, the mean interparticle distance can significantly exceed the characteristic length of the interaction potential, yielding solids and chain gases with densities several orders of magnitude lower than those of conventional quantum solids.

[1] G. Guijarro, G. E. Astrakharchik, G. Morigi, and J. Boronat, *Phys. Rev. Lett.* 133, 233402 (2024).

Hot Topic Talk, Tuesday 12:20-12:40, Saal Tirol

Stabilisation of spin mixtures and bound state spectroscopy in dipolar gases

Maxime Lecomte¹; Alexandre Journeaux¹; Julie Veschambre¹; Jean Dalibard²; Raphael Lopes³

¹ Laboratoire Kastler Brossel - ENS

² Laboratoire Kastler Brossel - Collège de France

³ Laboratoire Kastler Brossel - CNRS

Mixtures of ultracold gases with long-range interactions are expected to open new avenues in the study of quantum matter. Natural candidates for this research are spin mixtures of atomic species with large magnetic moments. However, the lifetime of such assemblies can be strongly affected by the dipolar relaxation that occurs in spin-flip collisions. Here we present experimental results for a mixture composed of the two lowest Zeeman states of ¹⁶²Dy atoms, that act as dark states with respect to a light-induced quadratic Zeeman effect. We show that, due to an interference phenomenon, the rate for such inelastic processes is dramatically reduced with respect to the Wigner threshold law [1]. Additionally, we determine the scattering lengths characterizing the $\mathbb{X}$ -wave interaction between these states, providing all necessary data to predict the miscibility range of the mixture, depending on its dimensionality. Looking ahead, our setup is a promising platform for studying supersolidity, including the formation of the so-called double supersolid [2].

Moreover, by exploiting spin-dependent light shifts, we probe several dimer bound states with binding energies as low as a few MHz across a magnetic field range of 0–20 G. These preliminary results reveal intriguing features in the collisional properties of dipolar gases.

[1] M. Lecomte, A. Journeaux, J. Veschambre, J. Dalibard and R. Lopes *PRL* 134, 013402, 2025

[2] D. Scheiermann, A. Gallemí, and L. Santos, “Excitation spectrum of a double supersolid in a trapped dipolar Bose mixture,” *arXiv:2412.05215*, 2024.

Collisions 2

Invited Talk, Tuesday 10:30-11:00, Saal Brüssel

Ion processing of astrophysically relevant molecular systems

Alicja Domaracka¹; Hermann Rothard¹; Philippe Boduch²

¹ CNRS-CIMAP

² UNICAEN-CIMAP

Astrophysical ices, mainly composed of simple molecules such as H₂O, CO, CO₂, NH₃, CH₃OH and others are ubiquitous in space: they are present in comets, satellites of planets (e.g. Jovian moons) and on the grains of the dense molecular clouds in the interstellar medium. They are constantly exposed to complex and diverse radiation fields and interact with photons, electrons and ions (solar/stellar winds, magnetospheres or/and cosmic rays). This induces several physico-chemical processes such as radiolysis and subsequent formation of new molecules, release of molecules to the gas phase (sputtering, desorption) and structural ice modifications.

During the talk, I will present an overview of results obtained for ion irradiation of ices containing small molecules as well as films of complex organic molecules (e.g. PAHs, nucleobases) performed with the “space

simulator” device IGLIAS at CIMAP using GANIL (Caen, France) ion beams. Additional experiments were performed at ATOMKI (Debrecen, Hungary) and GSI (Darmstadt, Germany). Infrared absorption spectroscopy is used to in situ observation of physico-chemical modifications of the icy layers during energetic processing. Ex-situ analysis of residues is performed by e.g. high resolution mass spectrometric methods. Astrophysical application of obtained results will be discussed. Moreover, the MIRRPLA platform will be also presented. MIRRPLA is a unique multibeam irradiation platform (UV photons, keV electrons and keV-GeV ions), which is under construction at CIMAP laboratory, to investigate the origin and evolution of organic matter of the Solar System. This project is financed by ANR PEPR (“Programmes et équipements prioritaires de recherche”) “Origins ».

Invited Talk, Tuesday 11:00-11:30, Saal Brüssel

Electron collisions with internally cold molecular ions in the Cryogenic Storage Ring

Oldrich Novotny

Max-Planck-Institut für Kernphysik

Collisions of molecular ions with electrons, such as dissociative recombination (DR) and inelastic electron collisions, play a key role in shaping the charge density and composition of cold plasmas, including the interstellar medium (ISM). Accurate rate coefficients are essential for modeling these astrophysical environments, yet theoretical calculations remain challenging due to the complexity of the underlying quantum dynamics. Experimentally, obtaining data at ISM-relevant conditions—collision temperatures of 10–100 K and low internal excitation—has been difficult. While previous storage ring studies reached the required collision temperatures, they struggled to achieve internal excitation temperatures below 300 K. This limitation has been overcome with the development of electrostatic cryogenic storage rings.

The Cryogenic Storage Ring (CSR) at the Max Planck Institute for Nuclear Physics in Heidelberg is a state-of-the-art electrostatic facility designed for studies with stored atomic, molecular, and cluster ion beams. Its cryogenic chamber operates at temperatures below 6 K, ensuring exceptionally low residual gas densities and enabling beam lifetimes of hundreds to thousands of seconds. For many molecular ions, this is sufficient time to relax into their lowest ro-vibrational states through spontaneous photon emission.

By replicating the extreme conditions of the cold ISM, CSR provides a unique platform for laboratory astrochemistry and quantum dynamics studies with well-defined molecular states. This talk will present recent CSR measurements on electron recombination of molecular ions in their lowest rotational states, with a focus on the unusual recombination behavior observed for TiO^+ , ArH^+ , and fullerenes.

- [1] R. von Hahn et al., Rev. Sci. Instr. 87, 063115 (2016)
- [2] O. Novotný et al., Science, 365, 676 (2019)
- [3] N. Jain et al., J. Chem. Phys. 158, 144305 (2023)
- [4] Á. Kálosi et al., Phys. Rev. A 110, 022816 (2024)

Invited Talk, Tuesday 11:30-12:00, Saal Brüssel

Cooling and colliding oppositely charged ions

Henning Zettergren

Stockholm University

The cryogenically cooled ion beam storage ring facility DESIREE (Double ElectroStatic Ion Ring Experiment) is uniquely designed for study-

ing mutual neutralization (MN) reactions in collisions between oppositely charged ions that are prepared in well-defined or narrow ranges of quantum states and with fine-control of the collision energy down to the sub-electronvolt regime [1,2]. In recent years, this has allowed a range of studies in which the final-state excitation energy distributions in atomic MN have been measured [3] and for the first ever MN studies with cooled molecular ions [4-6]. Such reactions are expected to be important for the ionization balance in any dilute environment where atomic or molecular anions are prominent negative charge carriers. Furthermore, the excellent vacuum conditions in DESIREE allows studying the cooling dynamics and stabilities of molecular ions on timescales exceeding minutes and in unprecedented detail [7-9].

This presentation will highlight recent DESIREE studies with a focus on complex molecular ions such as fullerenes, polycyclic aromatic hydrocarbons (PAHs), and biomolecules. These are important to benchmark theory and models that may be used for determining survival probabilities when molecules are exposed to different types of excitation agents in e.g. various interstellar environments, and for reliable predictions of MN rates that are expected to strongly influence the charge balance and hence the chemistry in dark interstellar clouds [10,11]. In addition, the MN studies reveal the importance of energy transfer, bond-breaking and bond-forming reactions in head-on collisions, which are driven by the Coulomb force between the oppositely charged ions. Here, support from quantum chemistry calculations is key to advance the understanding of such reactive charge transfer processes and to obtain accurate values of their rates.

References

- [1] R. D. Thomas et al, Review Scientific Instruments 82, 0655112 (2011).
- [2] H. T. Schmidt et al, Review Scientific Instruments 84, 055115 (2013).
- [3] See e.g. J. Grumer et al, Physical Review Letters 128, 033401 (2022) and references therein.
- [4] M. Poline et al, Physical Review Letters 132, 023001 (2024).
- [5] A. Bogot et al, Science 383, 285-289 (2024).
- [6] M. Gatchell et al, Astronomy & Astrophysics 694, A43 (2025).
- [7] M. Gatchell et al, Nature Communications 12, 6646 (2021).
- [8] P K Najeeb et al. Physical Review Letters 131, 113003 (2023).
- [9] M. Stockett et al, Nature Communications. 14 395 (2023).
- [10] S. Lepp and A Dalgarno, ApJ. 324, 553 (1988).
- [11] V. Wakelam and E. Herbst, ApJ. 680, 371 (2008).

Hot Topic Talk, Tuesday 12:00-12:20, Saal Brüssel

Laser-induced ionization triggers correlation-driven charge migration

Clément Guiot du Doignon; Rajarshi Sinha-Roy; Franck Rabilloud; Victor Despré

Universite Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, UMR5306, F-69100, Villeurbanne, France

In a molecular system, the correlation-driven charge migration [1] (CDCM) is a purely electronic process that involves the ultrafast dynamics of electrons originating from coherent superposition of eigenstates followed by the ionization of a single molecular orbital [2]. The possibility of observing CDCM has been a driving force behind theoretical and experimental developments in the field of attosecond molecular science since its inception. Although X-ray free-electron lasers (XFELs) have recently emerged as a promising tool for experimentally observing CDCM, the unambiguous observation of CDCM, or more generally, charge migration dynamics triggered by ionization, remains elusive. In this work [3], we present a method to selectively trigger such dynamics using molecules predicted to exhibit long-lived electron coherence. We show that these dynamics can be selectively triggered using infrared multi-photon ionization and probed using the spacial resolution of X-ray free-electron laser, proposing a promising experimental scheme to study these pivotal dynamics. Additionally,

we demonstrate that real-time time-dependent density-functional theory can describe correlation-driven charge migration resulting from a hole-mixing structure involving the HOMO of a molecule.

References

- [1] A. I. Kuleff, L. S. Cederbaum, J. Phys. B: At. Mol. Opt. Phys., **47**(12), 124002, (2014).
- [2] J. Breidbach, L. S. Cederbaum, J. Chem. Phys., **118**(9), 3983, (2003)
- [3] C. Guiot du Doignon, R. Sinha-Roy, F. Rabilloud, V. Despré, arXiv:2410.04978, (2024)

Hot Topic Talk, Tuesday 12:20-12:40, Saal Brüssel

Ultrafast correlation dynamics during high-harmonic generation in multi-electron atoms

Katharina Buczolic¹; Takeshi Sato²; Kenichi L. Ishikawa²; Fabian Lackner¹; Joachim Burgdörfer¹; Iva Březinová¹

¹ Institute for Theoretical Physics, Vienna University of Technology, 1040 Vienna, Austria, EU

² Graduate School of Engineering and Photon Science Center, School of Engineering, The University of Tokyo and Research Institute for Photon Science and Laser Technology, The University of Tokyo

We study the role of electronic correlations during high harmonic generation (HHG) in multi-electron atoms. Originally viewed as a process involving one single active electron, the influence of multi-electron effects on the HHG spectrum has lately been extensively studied (see e.g. [1, 2]). We quantify the time-dependence of electron-electron correlations on ultrafast time scales using correlation measures from quantum information theory.

By explicitly solving the time-dependent Schrödinger equation with the multi-configurational time-dependent Hartree-Fock (MCTDHF) method [3], we obtain fully correlated results for He, Ne, Be and Mg. Using driving fields adjusted to the ionization potential of each atom, such that the driving occurs in the strong-field regime and double-ionization is negligible, we compare the HHG yields for the different atomic species.

We find prominent features of the influence of correlations on both the tunneling as well as the recombination step. While during tunneling the correlations systematically increase for noble gas atoms (He, Ne), they decrease for alkaline earth atoms (Be, Mg). During recombination we find that the correlated electrons oscillate out of phase relative to each other. Both processes imprint distinct signatures of correlations on the HHG spectrum.

- [1] A. D. Shiner *et al.*, Nature Phys **7**, 464–467 (2011).
- [2] Y. Li *et al.*, Phys. Rev. A **99**, 043401 (2019).
- [3] T. Sato *et al.*, Phys. Rev. A **94**, 023405 (2016).

Fundamental 1

Invited Talk, Tuesday 17:00-17:30, Saal Straßburg

Precision Spectroscopy in Ion Coulomb Crystals and Search for New Physics

Tanja Mehlstäubler

PTB and Leibniz Universität Hannover

Trapped and laser-cooled ions allow for a high degree of control of atomic quantum systems. They are the basis for modern atomic clocks, quantum computers and quantum simulators. In our research we use ion Coulomb crystals, i.e. many-body systems with complex dynamics, for precision spectroscopy. This paves the way to novel optical ion frequency standards with ultra-high stability and accuracy for applications such as relativistic geodesy and quantum simulators in which complex dynamics become accessible with atomic resolution.

On the other hand, the high precision obtained in the spectroscopy of trapped cold ions enables sensitive tests of the Standard Model and the search for new physics. The long-lived F-state of the Yb⁺-ion has a high sensitivity to both relativistic and nuclear effects. We use isotope-shift spectroscopy as a sensitive probe for nuclear structure and fifth forces mediated by a new boson that couples to electrons and neutrons. Deviations from a linear relation in the King-plot analysis can indicate new physics or higher-order SM effects. This powerful technique revealed large King-plot nonlinearities in Yb. We present two-orders-of-magnitude improved spectroscopic measurements in all five stable spinless isotopes of this element. The transition frequency of the forbidden 2S_{1/2} to 2D_{5/2} and 2S_{1/2} to 2F_{7/2} transitions are determined with an accuracy of 6 and 16 Hz, respectively, yielding isotope shifts with a relative precision as low as 10⁻⁹. We combine these spectroscopic results with new mass measurements with a relative precision of a few 10⁻¹². With this, we can extract a new bound on the mass and coupling strength of the potential new bosons. The results are also used to investigate higher-order nuclear structure effects along a chain of Yb isotopes. In combination with ab initio nuclear structure calculations, this provides a window to nuclear deformation and nuclear charge distributions along isotopic chains towards exotic, neutron-rich nuclei.

Invited Talk, Tuesday 17:30-18:00, Saal Straßburg

High-resolution spectroscopy of molecular hydrogen ions

Jean-Philippe Karr

Laboratoire Kastler Brossel (Sorbonne Université, CNRS)

In the latest adjustment of fundamental constants [1], spectroscopy of ro-vibrational transitions in the molecular hydrogen ion HD⁺ contributed for the first time to the determination of particle masses, in particular the proton-electron mass ratio m_p/m_e , the precision of which was improved by a factor of 3.5. It was also used to constrain hypothetical beyond-standard-model interactions [2,3].

After reviewing the recent experimental and theoretical advances that led to these results, I will describe ongoing work towards improving further the theoretical accuracy by calculating certain QED corrections in a fully relativistic framework, relying on a high-precision numerical resolution of the Dirac equation for the bound electron [4]. Finally, perspectives for improved determination of fundamental constants offered by extending spectroscopic measurements to other isotopologues of the molecular hydrogen ion family (H₂⁺, D₂⁺, ...) will be discussed [5].

- [1] P. J. Mohr, D. B. Newell, B. N. Taylor, and E. Tiesinga, *arXiv:2409.03787*
- [2] M. Germann et al., *Phys. Rev. Research* 3, L022028 (2021).
- [3] C. Delaunay et al., *Phys. Rev. Lett.* 130, 121801 (2023).
- [4] H.D. Nogueira and J.-Ph. Karr, *Phys. Rev. A* 107, 042817 (2023).
- [5] S. Schiller and J.-Ph. Karr, *Phys. Rev. A* 109, 042825 (2024).

Invited Talk, Tuesday 18:00-18:30, Saal Straßburg

Trapped ions in optical tweezers

Rene Gerritsma

University of Amsterdam

Optical tweezers offer new opportunities to control and manipulate trapped ions with applications in quantum information processing, metrology and precision spectroscopy. The tweezers may be used to modify the local confinement of the ions, thereby modifying the sound-wave spectrum of the entire crystal. In this way, the soundwave mediated spin-spin interactions between the ions may be programmed with applications in quantum computing and simulation [1]. I will highlight our experimental progress towards implementing this system in the lab with emphasis on optimizing tweezer delivery and eliminating aberrations by using single ions as probes [2]. In the tightly focused tweezers, the paraxial approximation breaks down, leading to unexpected state-dependent forces on the ions in the direction perpendicular to the tweezers. I will explain how these may cause small, but avoidable errors in existing trapped ion quantum computing platforms and, conversely, how these may be used to our advantage for implementing novel quantum gates [3,4]. Finally, I will discuss our ideas of using the optical tweezers in precision spectroscopy.

- [1] J. D. Arias Espinoza et al., *Phys. Rev. A* **104**, 013302 (2021).
- [2] M. Mazzanti et al., *Phys. Rev. A* **110**, 043105 (2024).
- [3] M. Mazzanti et al., *Phys. Rev. Research* **5**, 033036 (2023).
- [4] L.P.H. Gallagher et al., *arXiv:2502.19345* (2025).

Ultracold 1

Invited Talk, Tuesday 17:00-17:30, Saal Tirol

Exploring the Roles of Nuclear Spins, Quantum Coherence, and Entanglement in Ultracold Chemistry

Kang-Kuen Ni

Harvard University

Coherence and entanglement are key features of quantum mechanics, although they are susceptible to environmental perturbations. A conventional strategy to entangle qubits with high fidelity is to leverage precisely controlled interactions while keeping qubits from decohering. By leveraging electric dipolar interactions, I will report entangling individual trapped NaCs molecules in optical tweezers and realizing a quantum logic gate with trapped molecules[1]. The bulk of the talk will try to go beyond this paradigm to explore and ask: Can coherence be preserved during chemical reactions and subsequently harnessed to produce entangled products? To address this question, we conduct investigations within the context of an atom-exchange chemical reaction ($2\text{KRb} \rightarrow \text{K}_2 + \text{Rb}_2$) at a temperature of 500nK[2]. I will share our research findings including surprises and puzzles.

- [1] Entanglement and iSWAP gate between molecular qubits, *Nature* 637, 821 (2025)

- [2] Quantum interference in atom-exchange reactions, *Science* 384, 1117 (2024)

Invited Talk, Tuesday 17:30-18:00, Saal Tirol

Ultracold highly magnetic and polar molecules for quantum simulation and new physics search

Michal Tomza

University of Warsaw

Ultracold mixtures involving highly magnetic atoms such as Er+Li, Dy+K, Cr+Li, and Er+Yb have already been realized for studying exotic quantum many-body phases. Such mixtures also open the way for the formation of ultracold diatomic molecules having both significant magnetic and electric dipole moments. Molecules involving atoms with large orbital angular momenta, such as Dy and Er, have a prohibitively complex internal structure with chaotic rovibrational spectra. In contrast, molecules involving highly magnetic symmetric atoms such as Cr or Eu may form exotic doubly polar molecules with easier-to-predict structures. On the other hand, molecules involving electronegative coinage metals such as Ag and alkali-metal atoms should possess very large permanent electric dipole moments.

In my talk, I will present several classes of highly polar and paramagnetic diatomic molecules, which can be produced at ultralow temperatures from laser-cooled ultracold atoms. I will show a new mechanism of useful Feshbach resonances in Cr+Yb mixtures [1] and the application of ground-state YbCr molecules for new physics searches [2], a recent experimental realization of weakly-bound LiCr molecules and our theoretical prediction of transferring them to the absolute ground state [3], as well as all-optical formation schemes of highly polar KAg and CsAg molecules [4]. Finally, I will discuss the possible application of ultracold highly polar and paramagnetic diatomic molecules in studying controlled collisions and chemical reactions and using them for precision measurements, quantum simulations, and quantum computing.

References:

- [1] M. D. Frye, P. S. Żuchowski, M. Tomza, *Phys. Rev. Research* 6, 023254 (2024)
- [2] A. Ciamei, A. Koza, M. Gronowski, M. Tomza, *arxiv* (2025)
- [3] S. Finelli, A. Ciamei, B. Restivo, M. Schemmer, M. Inguscio, A. Trenkwalder, K. Zaremba-Kopczyk, M. Gronowski, M. Tomza, M. Zaccanti, *PRX Quantum* 5, 020358 (2024)
- [4] M. Śmiałkowski, M. Tomza, *Phys. Rev. A* 103, 022802 (2021)

Invited Talk, Tuesday 18:00-18:30, Saal Tirol

Testing fundamental physics with ultracold molecules

Michael Tarbutt

Imperial College London

The most precise measurements of the electron's electric dipole moment (eEDM) all use molecules [1,2]. The molecules are spin polarized, and the eEDM determined by measuring the spin precession frequency in an applied electric field. The precession is due to the interaction of the eEDM with an effective electric field which can be exceptionally

large for heavy polar molecules. To reach high precision we need long spin precession times, which is only possible with neutral molecules if they are cooled to low temperatures. I will report progress towards an eEDM measurement using laser-cooled YbF molecules [3]. In one experiment, we produce a beam of molecules cooled to sub-Doppler temperatures in the two transverse directions and measure the spin precession frequency as the molecules fly. This experiment is operational, and I will present the sensitivity that we reach and our efforts to control systematic errors. I will also present our progress in producing very slow YbF molecules and trapping them, with the longer-term aim of making an eEDM measurement using molecules trapped in an optical lattice.

[1] V. Andreev et al., *Nature* 562, 355 (2018)

[2] T. S. Roussy et al., *Science* 381, 46 (2023)

[3] N. J. Fitch, J. Lim, E. A. Hinds, B. E. Sauer and M. R. Tarbutt., *Quantum Sci. Technol.* 6, 014006 (2021)

Ultrafast 2

Invited Talk, Tuesday 17:00-17:30, Saal Brüssel

Attosecond and few-femtosecond electron dynamics in photoexcited and photoionized organic molecules

Fernando Martin

Universidad Autonoma de Madrid and IMDEA Nanoscience

Light induced charge transfer in molecular complexes containing electron donor and acceptor groups is at the basis of organic photovoltaic devices. To capture the time evolution of this process at the early stages, ideally attosecond time-resolution is required. With the help of elaborate theoretical methods, attosecond pump-probe experiments allow one to image the motion of the “fast” electronic motion in these molecules, mostly in the gas phase, and understand how this motion affects the “slower” motion of atomic nuclei and vice versa. Currently, attosecond pulses produced by high harmonic generation inevitably lead to ionization, so that most of the reported studies concern electron dynamics generated in molecular cations [1-7]. But very recently, UV pulses of few-fs duration have become available [8,9], which combined with attosecond probe pulses, have opened the way to investigations of charge transfer dynamics in neutral molecules with attosecond resolution.

In this talk, I will present the results of theoretical simulations of attosecond pump-probe experiments to investigate the early stages of charge transfer in the donor-acceptor para-nitroaniline (PNA) and meta-nitroaniline (MNA) molecules, both in the neutral and cationic forms. The theoretical approach describes (i) the coherent excitation or ionization of the molecules by the pump pulse, (ii) the ensuing coupled electron and nuclear dynamics, and, in some cases, (iii) the time-resolved photoelectron spectra that should ideally be measured. The results show the strong interdependence between electronic and nuclear motions even during the first few femtoseconds of the charge dynamics.

[1] G. Sansone et al, *Nature* 465 763 (2010).

[2] F. Calegari et al, *Science* 346, 336 (2014).

[3] M. Nisoli, P. Decleva, F. Calegari, A. Palacios, and F. Martín, *Chem. Rev.* 117, 10760 (2017).

[4] F. Calegari and F. Martín, *Commun. Chem.* 6, 184 (2023).

[5] A. Palacios and F. Martín, *WIREs Comput. Mol. Sci.* e1430 (2020).

[6] G. Grell et al, *Phys. Rev. Res.* 5, 023092 (2023).

[7] F. Vismarra et al, *Nature Chemistry* 16, 2017 (2024).

[8] M. Galli et al, *Optics Letters* 44, 1308 (2019).

[9] M. Reduzzi et al, *Optics Express* 31, 26854 (2023).

Invited Talk, Tuesday 17:30-18:00, Saal Brüssel

Controlling entanglement and the forces on the nuclei with atto and few femto-second pulses

Francoise Remacle

University of Liege, Department of Chemistry, Belgium

The broad energy bandwidth of ultrashort pulses enables building a coherent superposition of electronic states. As a result, the electronic density is out of equilibrium and its localization between nuclei can be controlled on a purely electronic time scale.[1] As the nuclei begin to move, the electronic and nuclear motions are entangled.[2] This entanglement can be usefully exploited for controlling the force exerted by the vibronic wave packet on the nuclei [3] and steering chemical reactivity for bond making and fragmentation.[4,5] The dynamics of entanglement will be discussed for oriented molecules: The photoexcited bound N₂ molecule and the LiH molecule whose excited states are dissociating. The role of entanglement will be then discussed in polyatomic molecules undergoing structural rearrangements: Bond making in the photoinduced isomerization of norbornadiene into quadricyclane(4), the structural Jahn-Teller rearrangement of the methane cation upon sudden photoionization(5). Control schemes exploiting electronic coherences are not limited to oriented the molecules. We will show that it can be implemented in ensemble of molecules with initial random orientations with respect to the pulse polarization. The principal orientations of the ensemble are characterized using Singular Value Decomposition (SVD).[6] SVD provides insights on the stereodynamics. The approach will be illustrated for the case of an ensemble of initially randomly oriented LiH molecules photoexcited by a short CEP controlled IR pulse and for the forces driving the ultrafast Jahn-Teller (JT) structural rearrangement of the methane cation induced by XUV photoionization.

[1]. F. Remacle et al *Proc. Natl. Acad. Sci. USA* 103, 6793 (2006).

[2]. M. Blavier et al *Phys. Chem. Chem. Phys.* 24, 17516 (2022).

[3]. M. Cardosa et al *J. Phys. B* 57, 133501(2024).

[4]. A. Valentini et al *Phys. Chem. Chem. Phys.* 22, 22302 (2020).

[5]. C.E.M. Gonçalves, et al *Phys. Chem. Chem. Phys.* 23 12051 (2021).

[6]. M. Cardosa et al *J. Phys. Chem. A* 128, 2937 (2024).

Invited Talk, Tuesday 18:00-18:30, Saal Brüssel

Watching a molecular bond break

Tian Wang¹; Nida Haram²; Zack Dube²; Kyle Hamer³;
Yonghao Mi²; Caterina Vozzi⁴; Michael Schuurman⁵;
Nicolas Douguet³; David M. Villeneuve²; Paul B.
Corkum²; Andre Staudte²

¹ University of Ottawa, State Key Laboratory of Magnetic Resonance and Atomic and Molecular Physics, Wuhan Institute of Physics and Mathematics, Wuhan 430071, China

² National Research Council of Canada, University of Ottawa

³ University of Central Florida

⁴ CNR IFN { Istituto di Fotonica e Nanotecnologie, Piazza Leonardo da Vinci 32, 20133 Milan, Italy

⁵ National Research Council of Canada

The coupled motion of electrons and nuclei is central to understanding fundamental processes in molecules. Here, we investigate the ultrafast photodissociation of bromine (Br₂) using a femtosecond pump-probe scheme [1]. In our experiment a weak 400 nm pulse initiates dissociation along the neutral C-state, followed by an 800 nm probe pulse that ionizes the evolving fragments at variable delay. We detect the three-dimensional momenta of both photoions and photoelectrons in coincidence using COLD Target Recoil Ion Momentum Spectroscopy

(COLTRIMS) [2], in order to correlate the internuclear distance with the transition from a molecule to two separate atoms.

Positive delays mean that the intense, 800 nm probe pulse arrives after the pump pulse. Coulomb explosion is used to infer the internuclear distance in the single ionization channel which is correlated to the photoelectron momentum distributions.

Our measurements reveal a clear transition from molecular-like ionization channels at short pump-probe delays to atom-like channels at longer delays. The extracted photoelectron distributions show the evolution of valence orbitals from Br₂-centered wavefunctions to Br atomic orbitals as the internuclear distance increases. Numerical simulations using semiclassical two-step (SCTS) modeling and time-dependent density functional theory corroborate that a redistribution of ion core charge drives these characteristic momentum features [3].

By comparing ion kinetic energy release with the molecular-frame photoelectron momentum distributions, we find that the electronic evolution precedes the full separation by about 50 fs, emphasizing the significance of electron-nuclear coupling [1]. These findings highlight the need for multi-observable approaches to disentangle parallel electronic and structural rearrangements, thereby clarifying benchmark timescales for chemical bond cleavage.

References

- [1] W. Li et al. 2010 PNAS 107 20219
- [2] J. Ullrich et al. 2003 Rep. Prog. Phys. 66 1463
- [3] T. Wang et al. 2025 in preparation

Ultrafast 3

Invited Talk, Thursday 10:30-11:00, Saal Straßburg

Attosecond electron dynamics in solutions

Mette Gaarde

Louisiana State University

Attosecond science addresses the dynamics of electrons on their natural time scale, and much progress has been made in the understanding of processes such as attosecond charge migration; attosecond photoionization times; and the driven attosecond dynamics that takes place during high-harmonic generation (HHG). The majority of attosecond studies have been performed on atoms and molecules in the gas phase, with recent extensions of HHG into crystalline solids. However, many organic molecules of interest exist most naturally in the liquid phase, and only a few studies have emerged on the influence of a liquid environment on the initiation, evolution, and probing of attosecond dynamics.

In this talk I will report on two recent efforts studying attosecond dynamics in solutions, in which a low concentration of a molecule of interest is mixed into a liquid solvent: (i) We have compared core-hole-initiated charge migration in fluoroaniline in different solutions, using time-dependent density functional theory calculations. We find that the charge migration period, which is less than 1 fs, stays relatively constant independent of the solvent. However, in the solutions we find finite dephasing times for the dynamics that depend strongly on the solvent, suggesting that solute-solvent interactions indeed have an influence on the attosecond electron dynamics. (ii) In a joint experiment-theory work, we have studied HHG in different solutions of halobenzenes (PhX) and methanol (MeOH). Our experimental results show evidence of local order in the solvation of fluorobenzene (PhF) in MeOH. This manifests as a near-complete suppression of a single harmonic in the solution, which is absent in each of the pure liquids and absent in other PhX-MeOH solutions. We interpret the results in terms of a solvation shell that is formed in the PhF-MeOH solution and acts like a local barrier in the HHG process.

Invited Talk, Thursday 11:00-11:30, Saal Straßburg

X-ray induced Coulomb explosion images quantum fluctuations and reaction dynamics in complex molecules

Rebecca Boll

European XFEL

Coulomb explosion imaging (CEI) of polyatomic molecules induced by intense, femtosecond pulses at the European X-ray free-electron laser (EuXFEL) has allowed several new insights. In recent years, CEI has resolved asymmetric deformation and bond-angle opening in fragmenting water molecules [Jahnke2021], reconstructed the three-dimensional geometry of a five-atom molecule using a charge buildup model [Li2021, Li2022], and imaged a complex eleven-atom molecule—including all hydrogen atoms—while tracing intramolecular electron transfer [Boll2022]. More recently, CEI has captured the time-resolved deplanarization reaction following UV excitation of a heterocycle [Jahnke2025].

The multidimensional nature of CEI allows selective investigation of complex structural dynamics. Here, we demonstrate how X-ray induced CEI can be used to trace the correlated dynamics of a molecular elimination reaction—a minor reaction pathway involving the cleavage of two bonds and the formation of a vibrationally excited di-halogen fragment [Li2025]. In parallel, we map the light-induced bending vibration of the bound molecular wave packet and disentangle competing dissociation channels.

As CEI advances toward more quantitative structural analysis, interpretation becomes increasingly complex. Previous studies have relied on molecule-specific data processing tailored to each system and science case. To establish CEI as a more general and broadly applicable method, systematic approaches for analyzing high-dimensional ion-coincidence data are needed, as some quantitative insights can only be obtained through comparison with advanced modelling. Recent efforts in this direction include the application of principal component analysis (PCA) to simulated CEI data [Richard2021]. Building on this, we have now applied PCA to experimental data for the first time, overcoming significant technical challenges. This analysis enabled the extraction of collective ground-state structural fluctuations (zero-point motion) in a complex molecule [Richard2025]. To our knowledge, this represents the first direct experimental observation of this fundamental quantum phenomenon in a system of comparable complexity. The zero-point motion manifests as correlated variations in ion momenta, establishing CEI as a powerful tool for accessing high-dimensional quantum dynamics.

References

- [Boll2022] R. Boll et al., Nat. Phys. 18, 423 (2022)
- [Jahnke2021] T. Jahnke et al., Phys. Rev. X 11, 041044 (2021)
- [Jahnke2025] T. Jahnke et al., Nat. Commun. 16, 2074 (2025)
- [Li2021] X. Li, R. Boll, D. Rolles and A. Rudenko, Phys. Rev. A 104, 033115 (2021)
- [Li2022] X. Li et al., Phys. Rev. Res. 4, 013029 (2022)
- [Li2025] X. Li et al., Imaging a Light-Induced Molecular Elimination Reaction with an X-ray Free-Electron Laser, under review (2025)
- [Richard2021] B. Richard et al., Journal of Physics B 54, 194001 (2021)
- [Richard2025] B. Richard et al., Imaging collective quantum fluctuations of the structure of a complex molecule, under review (2025)

Invited Talk, Thursday 11:30-12:00, Saal Straßburg

Generating quantum entanglement using intense XUV-pulses from free-electron lasers

Saikat Nandi

Institut Lumière Matière, CNRS

When two or more quantum particles in a many-body system are entangled, its wavefunction cannot be factorized as a product of the wavefunctions of its constituents. It has been central to the ongoing second quantum revolution, as seen in the rapid development of the quantum information science. Initially, the idea of entanglement was dismissed by Albert Einstein himself as the ‘spooky’ action-at-a-distance. However, as it turned out, the photoelectric effect itself presents a unique opportunity to study the quantum entanglement between the emitted photoelectron and the residual ion – measurement of the kinetic energy of the former determines the exact quantum state of the later. Here, using intense extreme ultraviolet (XUV) pulses from a seeded free-electron laser, FERMI [1], we generate quantum entanglement between a photoelectron wave-packet rapidly expanding in space and a hybrid light-matter system, namely, a He⁺ ion dressed with an XUV photon. In the presence of the entanglement between these two massive particles, the measured photoelectron spectra clearly show an avoided crossing reminiscent of the Rabi cycling in the XUV-dressed residual ion [2]. In the absence of entanglement, however, the measured kinetic energies of the photoelectrons increase monotonically with increase in the photon energy, as predicted by Einstein’s photoelectric equation. We show that even if the photoelectron wave-packet expands up to a mesoscopic distance of almost 200 nm [3], it still remains entangled to the residual ion. Our results offer opportunities to explore quantum entanglement across ultrafast timescales over macroscopic distances.

References:

- [1] E. Allaria et al., Highly coherent and stable pulses from the FERMI seeded free-electron laser in the extreme ultraviolet. *Nature Photonics* 6, 699 (2012).
- [2] S. Nandi et al., Observation of Rabi dynamics with a short-wavelength free-electron laser. *Nature* 608, 488 (2022).
- [3] S. Nandi et al., Generation of entanglement using a short-wavelength seeded free-electron. *Science Advances* 10, eado0668 (2024).

Hot Topic Talk, Thursday 12:00-12:20, Saal Straßburg

Spectroscopic measurements of the Rydberg-surface Casimir-Polder Interaction

Esther Butery¹; Chris Boldt²; Biplab Dutta¹; Paolo Pedri¹; Stefan Scheel²; Athanasios Laliotis¹

¹ Université Sorbonne Paris Nord

² Universität Rostock

Highly excited (Rydberg) atoms have exaggerated properties making them extremely sensitive to external electromagnetic fields and interacting strongly with their environment. Atomic vapor cells represent an attractive platform for studying Rydberg atoms and fabricating quantum devices. For example, Rydberg atoms in vapor cells have been used as sensitive detectors of electric fields of frequencies ranging from DC up to the THz range but also as single photon sources for quantum technology applications exploiting collective phenomena due to the Rydberg blockade effect [1].

Rydberg atoms also find applications in fundamental physics, in particular for the measurement of dispersive interactions of the Casimir-Polder type (atom-surface interactions) [2] or of the van der Waals type (atom-atom interactions). One major advantage of Rydberg atoms is

that they expose limitations in the traditional perturbative approach of Casimir-Polder (CP) theory [3, 4]. Indeed, in the extreme near-field (i.e. when the atomic radius is no longer negligible compared to the atom-surface distance), the dipole approximation breaks down and higher-order terms need to be considered. Our recent theoretical study on Rydberg-surface interactions has provided calculations of the dipole-dipole terms that scale as $-C_3/z^3$ as well as quadrupole-quadrupole and dipole-octupole terms that scale as $-C_5/z^5$, clearly demonstrating that higher order terms could be experimentally relevant in vapor nanocell spectroscopy [4].

We report on extensive experimental measurements of the Rydberg-surface interaction using spectroscopy in cesium vapor nanocells of a thickness ranging roughly from 200-700nm, as well as selective reflection spectroscopy on a macroscopic cesium all-sapphire cell. Atoms are first excited to the Cs($6P_{1/2}$) level with a 894nm pump laser and subsequently a green laser $\approx$ 510nm probes Rydberg $nD_{3/2}$ or $nS_{1/2}$ states, where the principal quantum number n ranges between 15-17. Our experiments evidence the dipole-dipole term of the Casimir-Polder interaction providing a measurement of the C_3 coefficient for cesium Rydberg states. Furthermore, our experiment clearly evidences an additional interaction that induces shifts and broadens the linewidth of the probed transitions in the vicinity of the dielectric windows of our cells. We believe that this interaction is due to electric fields that are either generated by patch charges (trapped on the surface or induced by the excitation lasers), or by cesium adsorbants. We show that the different polarizability (of opposing sign) between S and D Rydberg states can be exploited to extract quantitative measurements of the strength and distance scaling (z-dependence) of such parasitic electrostatic interactions.

Our experiments suggest that the sensitivity of Rydberg atoms to external electric fields could provide a unique tool for probing electrostatic interactions in the vicinity of surfaces. This could allow systematic error corrections in Casimir-Polder experiments with excited or even ground state atoms that aim at putting bounds on the existence of non-Newtonian gravity [5]. We are currently exploring the possibility of coating the internal window interfaces with conducting 2D material such as graphene to reduce the influence of parasitic charges. This could allow us to probe atoms closer to the surface, at distances around 100nm, where quadrupole interactions (C_5 coefficient) could be experimentally attainable for the first time.

References

- [1] H. Kubler, J. P. Shaffer, T. Baluktsian, R. Loew, T. Pfau, *Nat. Photon.*, 4, 112–116 (2013).
- [2] V. Sandoghdar et al., *Phys. Rev. Lett* 68, 3432–3435 (1993).
- [3] J. A. Crosse et al., *Phys. Rev. A* 82, 3010901 (2010).
- [4] B. Dutta et al., *Phys. Rev. Res.* 6, L022035 (2024).
- [5] A. Laliotis, B-S. Lu, M. Ducloy, D. Wilkowski, *AVS Quantum Sci.* 3, 043501 (2021).

Hot Topic Talk, Thursday 12:20-12:40, Saal Straßburg

Advances in High-Mass Matter-Wave Interferometry

Stefan Gerlich

University of Vienna

Matter-wave interferometry serves as a fundamental test of quantum mechanics, directly probing the superposition principle and constraining potential modifications to the theory.

Recent experiments have demonstrated quantum interference of nanoparticles exceeding 25,000 Da [1], and the newest generation of interferometers aims to extend this mass limit by one to two orders of magnitude [2]. We present preliminary data from our new experimental setup, designed to observe interference of metal clusters at unprecedented mass scales of 100.000 Da and beyond.

Additionally, we explore applications of matter-wave interferometry in molecular metrology and discuss ongoing efforts to extend these

techniques to biomolecules, including proteins.

- [1] Y. Fein et al., *Nature Phys.* **15**, 1242, (2019)
 [2] F. Kialka et al., *AVS Quantum Sci.* **4**, 020502 (2022)

Spectroscopy 2

Invited Talk, Thursday 10:30-11:00, Saal Tirol

High resolution single molecule spectroscopy in a cryogenic ion trap

David Patterson

University of California, Santa Barbara

Single molecular ions present a highly attractive platform for high resolution and highly sensitive spectroscopy. These molecules can be held for many hours in a pristine environment, and can be motionally laser cooled into the millikelvin regime and below. Prior to this work, methods to study “generic” single molecular ions have not been demonstrated. Here, we demonstrate a novel single molecule action-spectroscopy technique that is compatible with high precision measurement, and present rotationally resolved spectra of single polyatomic ions. The method is generally applicable to a wide range of polyatomic molecular ions, and promises spectral resolution comparable to state of the art quantum logic methods, with significantly less stringent experimental overhead. Progress towards extending this technique to include chiral recognition of single molecules will be discussed. Adaptations of this technique will prove useful in a wide range of precision spectroscopy arenas including the search for parity violating effects in chiral molecules and searches for biological signatures in samples from beyond Earth.

Invited Talk, Thursday 11:00-11:30, Saal Tirol

Cavity-Enhanced Dispersive Interaction of Cold Atoms with an Optical Frequency Comb

Ticijana Ban¹; Ivor Krešić²; Marin Đujić¹

¹ Institute of Physics

² Institute of Physics

We report the first experimental realization of cold atoms interacting with an optical frequency comb (OFC) inside a high-finesse Fabry-Perot cavity in the dispersive regime. This is achieved by leveraging the narrow optical transition of the cold atoms, with a linewidth much smaller than the free spectral range of the cavity, allowing all cavity modes to be detuned far from atomic resonance and simultaneously excited by a multiple of frequency comb modes.

In the linear dispersive regime of light-matter interaction, we observe a collective frequency shift of multiple cavity modes in the spectrum of the transmitted OFC. In the nonlinear regime, we study bistability in the transmission of a single comb mode, induced by optical pumping in Zeeman ground states.

These results introduce a new approach to controlling light-matter interactions with multiple OFC modes in cavity-enhanced setups, paving the way for the implementation of recent proposals in cavity cooling [1], quantum annealing [2, 3], and quantum simulations [4].

References:

- [1] Torggler, I. Krešić, T. Ban, and H. Ritsch, *New Journal of Physics* **22**, 063003 (2020).
 [2] V. Torggler, S. Krämer, and H. Ritsch, *Phys. Rev. A* **95**, 032310 (2017).
 [3] Torggler, P. Aumann, H. Ritsch, and W. Lechner, *Quantum* **3**, 149 (2019).
 [4] N. Masalaeva, H. Ritsch, and F. Mivehvar, *Phys. Rev. Lett.* **131**, 173401 (2023).

Invited Talk, Thursday 11:30-12:00, Saal Tirol

Spatio-temporal tailored attosecond light pulses for exploring ultrafast localized phenomena

Carlos Hernandez-Garcia

Universidad de Salamanca

The development of structured ultrafast laser sources has been crucial for advancing our understanding of the fundamental dynamics of electronic and spin processes in matter. In particular, ultrafast laser pulses structured in their spin angular momentum (linked to light polarization) and orbital angular momentum (related to the transverse phase profile or vorticity of a light beam) play a relevant role in studying chiral systems and magnetic materials at their intrinsic temporal and spatial scales.

Recent advancements have enabled the generation of structured ultrafast laser pulses on attosecond timescales, leading to significant progress in nonlinear optics. Specifically, the highly nonlinear process of high harmonic generation (HHG)—which up-converts an intense infrared driving beam into the extreme-ultraviolet (EUV) or soft X-ray region—now allows the creation of structured light pulses at the attosecond timescale.

This talk will review key developments in the field of attosecond structured pulses over the past decade [1-4], with a special focus on the up-conversion of spatio-spectral and spatiotemporal optical vortices [5]. These beams are particularly well-suited for probing ultrafast electronic dynamics in systems with coupled spatial and temporal responses. We shall explore potential applications of these structured attosecond pulses in investigating localized ultrafast phenomena across fundamental and applied science.

[1] C. Hernández-García, A. Picón, J. San Román, and L. Plaja “Attosecond extreme ultraviolet vortices from high-order harmonic generation” *Phys. Rev. Lett.* **111**, 083602, (2013).

[2] A. K. Pandey, et al., *ACS Photonics* **9** (3), 944-951 (2022)

[3] A. de las Heras, D. Schmidt, J. San Román, J. Serrano, J. Barolák, B. Ivanic, C. Clarke, N. Westlake, D. Adams, L. Plaja, C. G. Durfee, C. Hernández-García, “Attosecond vortex pulse trains”, *Optica* **11**, 1085 (2024).

[4] N. J. Brooks, A. de las Heras, B. Wang, I. Binnie, J. Serrano, J. San Román, L. Plaja, H. C. Kapteyn, C. Hernández-García, M. Murnane, “Circularly Polarized Attosecond Pulses enabled by an Azimuthal Phase and Polarization Grating”, *ACS Photonics* **12**, 1, 495-504 (2025).

[5] R. Martín-Hernández, G. Gui, L. Plaja, H. K. Kapteyn, M. M. Murnane, C.-T. Liao, M. A. Porras and C. Hernández-García. “Extreme-ultraviolet spatiotemporal vortices via high harmonic generation” *Nature Photonics*, in press (2025).

Hot Topic Talk, Thursday 12:00-12:20, Saal Tirol

Coherent nonlinear four X-ray photon interaction with core-shell electrons

Ana Sofia Morillo Candas¹; Sven Augustin²; Eduard Prat²; Antoine Sarracini²; Jonas Knurr²; Serhane Zerdane²; Zhibin Sun²; Ningchen Yang³; Marc Rebholz⁴; Hankai Zhang³; Yunpei Deng²; Xinhua Xie²; Andrea Cannizzo⁵; Andre Al-haddad²; Kirsten Schnorr²; Christian Ott⁴; Thomas Feurer⁶; Christoph Bostedt³; Thomas Pfeifer⁴; Gregor Knopp²

¹ Max-Planck-Institut für Kernphysik (MPIK, Max Planck Institute for Nuclear Physics)

² Paul Scherrer Institute

³ Paul Scherrer Institute, École Polytechnique Fédérale de Lausanne

⁴ Max-Planck-Institut für Kernphysik

⁵ University of Bern

⁶ University of Bern, European XFEL

1. Introduction

The X-ray spectral range can address atomic scale (nm) spatial resolution at ultrafast time (fs) scales, with element specificity and site-selective excitation. Non-linear wave mixing techniques in this range, in particular four-wave mixing (FWM) methods, can thus provide information on the structural and electronic dynamics of atomic and molecular systems with unprecedented resolution. X-ray FWM brings the capability to study the electronic states coupling between spatially localized inner and/or core transitions among different sites of a quantum system or to study transport phenomena at the nanoscale. Whereas mixed XUV/X-ray - optical four-wave mixing and all-EUV have been successfully demonstrated in a transient grating (TG) configuration (see refs. [1-3] and refs. therein), non-linear all-X-ray four-wave mixing spectroscopy has been envisioned and theoretically described [4] but not yet realized experimentally, remaining as a long-awaited goal until now [5].

We demonstrate nonlinear X-ray four-wave mixing (XFWM) will all photons in the soft X-ray range (850-870 eV) using a non-collinear folded 'Box' or BoxCARS configuration [6]. In this robust configuration and obeying phase-matching, the X-ray photons generated by three interacting soft X-ray beams are emitted towards the fourth corner of a square, allowing for background-free detection. The signal could thus be clearly discriminated from the incoming beams and detected either by an in-line X-ray grating spectrometer ($\Delta E \approx 0.4$ eV), allowing for its spectral characterization or by recording the fluorescence from a YAG screen moved into the signal beam path, for its spatial characterization.

2. Results

SASE pulses from the Swiss Free Electron Laser (SwissFEL) are focused by a pair of KB mirrors into an in-vacuum gas-cell filled with a few hundreds mbar of Ne producing a coherent response from core-shell electrons. When scanning the FEL pink beam available at the Maloja end-station around the Ne K-absorption edge at ~ 870 eV, the YAG fluorescence shows a laser-like signal beam, well isolated from the incoming beams, which shows the maximum signal strength when approaching the pre-edge resonances of Ne. The signal generation efficiency, as defined by the ratio of signal photons that are scattered into the phase-matched direction and the incoming photons is in the order of 0.15 %, demonstrating an efficient signal generation.

The spectrally dispersed XFWM signals provide a rich map, comprising multiple contributions from neutral neon and its ions. The large set of parameters explored, including FEL intensity, gas pressure and pulse duration ranging from 30 fs down to 3 fs (rms), provides key information that allow us to disentangle the different origin of the XFWM signals, including resonantly-enhanced X-ray two-color processes. The measured results are compared to the available literature on stimulated Raman X-ray scattering in Neon [7] and with the results of a dedicated model that accounts for the beam propagation and

population changes during the X-ray pulse duration. We discuss in detail the measured and calculated 2D spectral maps, and how the correlation plots reflect the coupling between electronic states of neon, allowing us to distinguish these signals from X-ray lasing processes originated in the ions.

The general feasibility of non-collinear four-wave mixing in the X-ray range is demonstrated. The robustness of the setup, the strength of the signals and the spectral and spatial information achieved from the experiment implies a major breakthrough for the application of nonlinear X-ray wave mixing as a spectroscopic tool in general, and as basis for 2D X-ray correlation spectroscopy. In addition, preliminary time resolved signals and approaches to extend the proposed methodology to the time domain, based on two-colour mode available at the Athos branch of SwissFEL are introduced.

3. References

- [1] F. Bencivenga et al., "Four-wave mixing experiments with extreme ultraviolet transient gratings" *Nature* 520, 205 (2015).
- [2] F. Bencivenga, et al. "Nanoscale transient gratings excited and probed by extreme ultraviolet femtosecond pulses." *Sci. Adv.* 5(7) eaaw5805 (2019).
- [3] J.R. Rouxel, D. Fainozzi, R. Mankowsky, B. Rösner, G. Seniutinas, et al. "Hard x-ray transient grating spectroscopy on bismuth germinate" *Nat. Photon* 15(7), 499–503 (2021)
- [4] S. Tanaka and S. Mukamel "X-ray four-wave mixing in molecules" *J. Chem. Phys.* 116(5), 1877–1891 (2002)
- [5] A.S. Morillo-Candas, et al. "Coherent all X-ray four-wave mixing at core shell resonances." *arXiv preprint arXiv:2408.11881* (2024), <https://doi.org/10.48550/arXiv.2408.11881>
- [6] Y. Prior, "Three-dimensional phase matching in four-wave mixing" *Appl. Opt.* 19(11), 1741–1743 (1980)
- [7] C. Weninger, M. Purvis, D. Ryan, R.A. London, J.D. Bozek, C. Bostedt, A. Graf, G. Brown, J.J. Rocca, and N. Rohringer, "Stimulated Electronic X-Ray Raman Scattering" *PRL* 111, 233902 (2013).

Hot Topic Talk, Thursday 12:20-12:40, Saal Tirol

Measurement of Single Photon Photoelectron Elliptical Dichroism of Electrosprayed Anions

Jon H. Both¹; Karl-Michael Weitzel²

¹ Philipps-Universität Marburg

² Philipps-Universität Marburg

Investigations aiming at the determination of molecular chirality by chiroptical techniques continue to attract a significant amount of interest in chemistry, physics biology and pharmacology. Some focus has been put on the measurement and analysis of the photo ion circular dichroism (PICD) –a total ion yield effect –and the Photoelectron Circular Dichroism (PECD) –a molecular frame angular distribution effect. Most efforts have put immense work into establishing "perfect" circular polarization.

In recent years it has been demonstrated, that Photoelectron Elliptical Dichroism (PEELD) –which considers a systematic variation of the elliptical polarization of light –is also a powerful approach for studying chirality. Basically, PEELD is the extension of PECD to a variation of elliptical polarization. So far, PEELD has been reported for a number of neutral analytes using multi photon ionization, demonstrating advantages over plain PECD experiments.[1,2,3] PEELD measurements with single photon ionization have not been reported yet, due to the comparably high ionization energy of neutral analytes.

In this work we demonstrate the measurement of PEELD in single photon photodetachment of electrons from electro-sprayed anions. Photodetachment of electrons from anions has recently been developed as a new technique for chirality analysis.[4,5,6,7] When combined with electro-spraying the anions of interest, the technique, ESI-PECD, allows the study of proteins containing many amino acids.[5]

As analytes we chose, amino acids, for which the quantification of enantiomeric excess has already been demonstrated by ESI-PECD in

our group, i.e. phenylalanine and tryptophan.[7] In this work, we show that the PEELD of the phenylalanine-anion scales linearly with the STOKES parameter S_3 for small values of S_3 . There is a distinct extremum of the PEELD in the region of $[S_3 / S_0] = 0.95$ with very good symmetry between D- and L-phenylalanine. We note, that there are literature reports indicating non-linear variation of the PEELD with S_3 , however, in the case of multi photon ionization.[1,2,3]

The study of PEELD in photodetachment is expected to shed new light on the fundamental question of asymmetry in the photoelectron angular distribution comparing multiphoton and single photon processes. It is argued that a well-defined elliptic polarization has to be preferred over an ill-defined circular polarization.

- [1] A. Comby, D. Descamps, S. Petit, E. Valzer, M. Wloch, L. Pouységu, S. Quideau, J. Bocková, C. Meinert, V. Blanchet, B. Fabre, Y. Mairesse, *Phys. Chem. Chem. Phys.* 2023, 25, 16246–16263.
- [2] A. Comby, E. Bloch, C. M. M. Bond, D. Descamps, J. Miles, S. Petit, S. Rozen, J. B. Greenwood, V. Blanchet, B. Fabre, Y. Mairesse, *Nat. Commun.* 2018, 9, 5212.
- [3] J. B. Greenwood, I. D. Williams, *Phys. Chem. Chem. Phys.* 2023, 25, 16238–16245.
- [4] P. Krüger, K.-M. Weitzel, *Angew. Chem. Int. Ed.*, 2021, 60, 17861–17865.
- [5] P. Krüger, J. H. Both, U. Linne, F. Chiro, K.-M. Weitzel, *J. Phys. Chem. Lett.*, 2022, 13, 6110–6116.
- [6] J. Triptow, A. Fielicke, G. Meijer, M. Green, *Angew. Chem. Int. Ed.*, 2022, 62, e202212020.
- [7] J. H. Both, A. Beliakouskaya, K.-M. Weitzel, *Analytical Chemistry*, 2025, in press, (<https://doi.org/10.1021/acs.analchem.4c05964>).

Ultracold 2

Invited Talk, Thursday 10:30-11:00, Saal Brüssel

Exploring Rydberg Atom Interactions Near Optical Nanofibres

Sile Nic Chormaic; Alexey Vylegzhanin; Anna Kortel; Aswathy Raj; Krishna Jadeja; Michelangelo Dondi; Pit Steinmetz; Sergei Abdrakhmanov; Wenfang Li; Zohreh Shahrabifarahani

OIST Graduate University

Optical trapping has transformed our ability to manipulate and control atoms and micro/nanoparticles, offering numerous applications and research directions across a wide range of scientific fields. From biological cells and colloidal microparticles to nanoparticles and cold atoms, the manipulation of single particles using optical tweezers has provided us with invaluable insights. One promising alternative to the conventional optical tweezers lies in the use of optical nanofibres - ultrathin fibres with a diameter smaller than the wavelength of light they are designed to guide. Such nanofibres confine light very tightly in the radially direction, creating an high intensity evanescent field beyond their glass boundary.

Advantageously, setups involving optical nanofibres tend to be simple and have a very small footprint, leading to “lab-on-chip” type applications. Within cold atom setups, they minimally disturb the magneto-optical trapping fields and provide an efficient data communication channel for directly sending or collecting light even down to the single photon level. With their strongly confined light fields, long interaction lengths, and low loss, nanofibres are excellent platforms for exploring phenomena like chiral atom-light interactions and waveguide quantum electrodynamics.

In our work, we have shown how Rydberg atom excitation can be mediated via an optical nanofibre, significantly reducing the power needed for the excitation to occur. We have also proposed trapping schemes for cold ground state and Rydberg state atoms by exploiting the evanescent field from optical nanofibres and combining it with a holographic tweezers configuration to create a hybrid atom trap platform. We will discuss our recent progresses, and also the limitations of this platform, during the talk.

Invited Talk, Thursday 11:00-11:30, Saal Brüssel

Hydrodynamics in an Ultracold Dipolar Gas

John Bohn

JILA, University of Colorado

Ultracold gases of paramagnetic atoms or dipolar molecules are fascinating in the quantum degenerate regime, to be sure. However, even a thermal gas consisting of these entities may have unusual features. Specifically, polar molecules with sufficiently large dipole moment can enter the hydrodynamic regime, where the mean-free path for collisions is far smaller than the scale of structures in the gas, for example, the wavelength of sound. In this circumstance it is plausible to consider the gas as a fluid, governed by Navier-Stokes type equations, but with the novelty that transport coefficients, such as heat conduction and viscosity, are anisotropic. I present a formulation of these equations and some preliminary results on sound modes as well as “weltering” dynamics that occurs in a trapped gaseous sample.

Invited Talk, Thursday 11:30-12:00, Saal Brüssel

Microscopy of strontium Bose- and Fermi-Hubbard systems

Carlos Gas¹; Sandra Buob¹; Jonatan Hörschele¹; Leonardo Bezzo¹; Vasiliy B. Makhlov¹; Antonio Rubio-Abadal¹; Leticia Tarruell²

¹ ICFO

² ICFO and ICREA

The development of quantum-gas microscopes has brought novel ways of probing quantum degenerate many-body systems at the single-atom level. Until now, most of these setups have focused on alkali atoms. Expanding quantum-gas microscopy to alkaline-earth elements as strontium will provide new tools, such as SU(2)-symmetric fermionic isotopes or ultranarrow optical transitions, to the field of quantum simulation.

In my talk, I will present our recent development of strontium quantum-gas microscopy, which enables imaging of both Bose- and Fermi-Hubbard systems in a single-atom and single-site resolved manner. All experiments are performed in an optical lattice operating at the clock-magic wavelength, which will allow us to exploit the clock transition in the future.

For bosonic strontium-84, we demonstrate single-atom resolved imaging of strontium lattice superfluids. In a first series of experiments, we realize fluorescence imaging using the broad 461-nm transition, which provides high spatial resolution, while simultaneously performing attractive Sisyphus cooling with the narrow 689-nm intercombination line. We reconstruct the atomic occupation from the fluorescence images, obtaining imaging fidelities above 94%. Exploiting instead the narrow intercombination line for both fluorescence collection and Sisyphus cooling allows us to enhance the fidelities to above 98% while

reducing the exposure time by an order of magnitude. Finally, we apply the narrow-line imaging scheme to fermionic strontium-87 and, exploiting the spectral selectivity of the intercombination line, demonstrate spin-resolved microscopy of a fermionic system with up to 10 internal states.

Our strontium quantum-gas microscope provides a new platform to study dissipative Hubbard models, quantum optics in atomic arrays, and SU(2) fermions at the microscopic level.

Hot Topic Talk, Thursday 12:00-12:20, Saal Brüssel

A cavity-microscope for micrometer-scale control of atom-photon interactions

Francesca Orsi; Rohit Prasad Bhatt; Ekaterina Fedotova; Michael Eichenberger; Léa Dubois; Jean-Philippe Brantut

EPFL

Cavity quantum electrodynamics studies the strong interaction between matter and the electromagnetic field of an optical cavity: the enhanced interaction is useful both for reading the properties of the atoms with a fast, sensitive and weakly destructive measurement and for quantum simulation where atoms interact by exchanging photons with each other at a distance. One of the drawbacks of these systems is the loss of spatial information that cavity-based measurement implies: the result of these measurements is an average of the properties of the atoms over the entire cavity field volume.

I will explain how we built and operated a cavity-microscope device that overcomes this problem: it realizes both a cavity and a pair of high numerical-aperture lenses in a single device and can be used to couple a microscopic part of the atomic cloud to the cavity field. We produce a cavity-based image of the atomic density by scanning the position of the microscope focus [1].

This technology opens the doors to analog quantum simulations of programmable, all-to-all interacting systems. I will report about the self-organization phase transition of a Fermi gas in a high-finesse cavity in the presence of tight confinement and the development of optical techniques to randomize cavity-mediated interactions. These interactions can drastically change the behavior of the system, and open the door to the exploration of models of holographic quantum matter such as the Sachdev-Ye-Kitaev model [2].

Hot Topic Talk, Thursday 12:20-12:40, Saal Brüssel

Collective light scattering in an array of dysprosium atoms

Britton Hofer; Damien Bloch; Giulio Biagioni; Nathan Bonvalet; Antoine Browaeys; Igor Ferrier-Barbut

Institut d'Optique

Dissipative quantum many-body problems, such as those arising in collective light-matter interactions, present theoretical challenges. To explore these phenomena experimentally, we have developed an experimental setup that studies collective light scattering from an ordered ensemble of atoms. Recently, we achieved the first trapping and imaging of single dysprosium atoms in optical tweezers [1], extending the single-atom toolbox to lanthanides. Leveraging the rich internal structure of dysprosium, we can measure the atoms' internal states which we use to investigate collective dissipation both in the linear optics regime and at high saturation [2]. To further enhance the collective

behavior of the atoms, we have two approaches. First, we cool the atoms close to their ground state using a 2 kHz transition [3]. Additionally, we are working to bring the atoms to a distance comparable to the wavelength of the transition used for light scattering by implementing a hybrid tweezer and accordion lattice setup.

[1] D. Bloch, B. Hofer, S. R. Cohen, A. Browaeys, and I. Ferrier-Barbut, *Trapping and imaging single dysprosium atoms in optical tweezer arrays*, Phys. Rev. Lett. 131, 203401 (2023)

[2] B. Hofer, D. Bloch, G. Biagioni, N. Bonvalet, A. Browaeys and I. Ferrier-Barbut, *Single-atom resolved collective spectroscopy of a one-dimensional atomic array*, arXiv:2412.02541 (2024)

[3] G. Biagioni et al. *Narrow line cooling of single dysprosium atoms*, in preparation

Ultracold 3

Invited Talk, Thursday 17:00-17:30, Saal Brüssel

Quantum continuous time crystals in neutral-atom arrays

Thomas Pohl

TU Wien

Continuous time crystals, i.e., nonequilibrium phases with a spontaneously broken continuous time-translational symmetry, have been studied and recently observed in the long-time dynamics of open quantum systems. In particular, experimental studies of strongly interacting thermal Rydberg gases have established that continuous time crystals (CTC) can emerge under the simultaneous optical driving of more than a single interacting Rydberg state [1].

Motivated by these results, we discuss in this talk the dynamics in lattices of interacting Rydberg atoms, under optical two-photon driving with a standard three-level ladder configuration. While the emergence of continuous time-crystal phases in open quantum system as typically based on an underlying mean-field phenomenology, we focus here on their formation under conditions that do not a priori justify a simplified meanfield treatment [2]. Using complementary numerical methods we find two distinct time-crystal phases that cannot be described within mean-field theory. Remarkably, one of these quantum continuous time crystals (qCTCs) emerges only in the presence of quantum fluctuations. Our findings extend explorations of continuous time-translational symmetry breaking in dissipative systems beyond the classical phenomenology of periodic orbits in a low-dimensional nonlinear system. Possible experiments to observe the predicted qCTC phases in tweezer arrays of neutral atoms are also discussed.

[1] X. Wu, Z. Wang, F. Yang et al., Dissipative time crystal in a strongly interacting Rydberg gas, Nature Physics 20, 1389 (2024)

[2] F. Russo and T. Pohl, Quantum Dissipative Continuous Time Crystals, arXiv:2503.16141 (2025)

Invited Talk, Thursday 17:30-18:00, Saal Brüssel

Thermal melting of a vortex lattice

Rishabh Sharma; David Rey; Laurent Longchambon;
Aurélien Perrin; Romain Dubessy; Hélène Perrin

Laboratoire de physique des lasers, Université Sorbonne Paris Nord and CNRS UMR7538

Quantum gases can be manipulated with a variety of experimental tools and offer an excellent platform for the study of superfluid dynamics. Superfluidity is characterized by a collection of intriguing dynamical behaviors, such as the existence of a critical velocity or the apparition of quantum vortices when the superfluid is set into rotation. At low temperature and moderate rotation frequency, these vortices form a crystalline phase and arrange into a triangular vortex lattice. As temperature or rotation increase, we observe a transition to a disordered phase for the vortex positions, and the vortex lattice melts. We study this phenomenon experimentally in a quasi two-dimensional quantum gas rotating at the bottom of a shell trap. We characterize the vortex phase by computing the position and angular correlations in the lattice for increasing rotation frequency, and compare our observation with the predictions of the Kosterlitz-Thouless-Halperin-Nelson-Young (KTHNY) theory for the thermal melting of a two-dimensional crystal through an hexatic phase.

Invited Talk, Thursday 18:00-18:30, Saal Brüssel

From Bose polarons to quantum droplets of light

Francesca Maria Marchetti

Universidad Autónoma de Madrid

Exciton-polaritons in 2D semiconductor heterostructures provide an ideal platform for exploring novel properties of strongly coupled light-matter quantum fluids. Recently, significant efforts have been dedicated to investigating beyond mean-field effects, with the long-term goal of entering the regime of quantum polaritonics. This presentation focuses on spinor polariton condensates, where, analogous to binary Bose mixtures in ultracold atomic systems, a bipolariton Feshbach resonance enables the realisation and study of beyond mean-field effects across various regimes—from the Bose polaron regime to the regime of self-bound polariton droplets, stabilized by a balance between mean-field interactions and quantum fluctuations.

Quantum 3

Invited Talk, Thursday 17:00-17:30, Saal Tirol

Quantum control of massive mechanical objects

Yiwen Chu

ETH Zürich

In recent years, it has become possible to control and the measure the quantum states of the motion of macroscopic mechanical objects. Such

efforts are motivated by both the study of fundamental science and the promise of new quantum technologies. I will give a brief overview of how recent advances in the fields of optomechanics and electromechanics have allowed us to explore the quantum behavior of solid-state mechanical objects and use them as new quantum resources. This will be followed by a few examples from my group's work on quantum control of bulk acoustic resonators and using them as sensors for new physics.

Invited Talk, Thursday 17:30-18:00, Saal Tirol

Non-Hermitian Skin Effect for Photon Pairs Interacting with Atom Arrays

Alexander Poddubny

Weizmann Institute of Science

Non-Hermitian skin effect (NHSE) has now become the paradigmatic example of the topologically nontrivial impact of loss or gain in optical and condensed matter systems. Here, I will present our latest theoretical results on an analog of NHSE in the platform of chiral waveguide quantum electrodynamics—the area of quantum optics studying interaction with propagating photons with atoms in a waveguide [1].

I will focus on the Non-Hermitian Skin effect for the bound states of interacting photons pairs propagating in a waveguide and chirally coupled to an array of atoms [2]. I will demonstrate the concentration of bound modes at the edge of the array that can be interpreted as a non-Hermitian skin effect. The mechanism behind this effect is rather unusual: contrary to the usual local loss or gain, the spectrum for the bound states in the infinite structure is lossless. Instead, the non-Hermiticity for bound pairs is driven by their dissociation into scattering states of photons in the finite structure. Unexpectedly, the bound pairs are concentrated at the left edge of the array when photons are preferentially emitted to the right, and vice versa.

The coexistence of the continuum with the quasiparticle dispersion branch is a generic feature for the energy spectra of various many-body systems, for example, with plasmonic or magnonic excitations. Thus, we believe that our results could apply beyond one-dimensional systems and beyond setups with atom-photon coupling.

[1] A. S. Sheremet, M. I. Petrov, I. V. Iorsh, A. V. Poshakinskiy, and A. N. Poddubny, Waveguide quantum electrodynamics: Collective radiation and photon-photon correlations, *Rev. Mod. Phys.* **95**, 015002 (2023).

[2] J. Shi and A.N. Poddubny, Chiral Dissociation of Bound Photon Pairs for a Non-Hermitian Skin Effect, arXiv:2501.09417

Hot Topic Talk, Thursday 18:00-18:20, Saal Tirol

Dissipative phase transitions with one and many atoms in cavities

András Vukics

HUN-REN Wigner Research Centre for Physics

I present the recent concept of first-order dissipative phase transitions, that can occur in meso- and even microscopic quantum systems.

One of the first examples of this phenomenon was the photon-blockade breakdown (PBB) effect, occurring most simply in the driven-dissipative Jaynes-Cummings model that contains only a single qubit. For PBB, an abstract thermodynamic limit has been identified [1]

where the coupling between the qubit and the mode goes to infinity without affecting the system size (a.k.a. zero-dimensional or finite-component phase transition). This limit was studied in a finite-size scaling approach [2], with scaling exponents determined numerically. PBB and its thermodynamic limit were observed in circuit QED systems [3,4]. For the highest realized coupling strength, the system alternates with a characteristic timescale as long as 6s –exceeding the microscopic timescales by 6 orders of magnitude –between a bright coherent state with approximately 10000 intracavity photons and the vacuum state.

In the second half of the talk, I describe analogous effects observed in a rubidium cold-atom cavity-QED setup [5]. Atoms in an optical cavity can manifest a first-order dissipative phase transition dubbed transmission-blockade breakdown. The stable coexisting phases are quantum states with high quantum purity, that include atomic hyperfine ground states and coherent states of electromagnetic field modes [6]. Similarly to PBB, the phases become perfectly pure states in the thermodynamic limit, making the phenomenon relevant for quantum technologies.

[1] Carmichael, Howard J. “Breakdown of photon blockade: A dissipative quantum phase transition in zero dimensions.” *Physical Review X* 5, no. 3 (2015): 031028.

[2] Vukics, András, András Domby, Johannes M. Fink, and Péter Domokos. “Finite-size scaling of the photon-blockade breakdown dissipative quantum phase transition.” *Quantum* 3 (2019): 150.

[3] Fink, Johannes M., András Domby, András Vukics, Andreas Wallraff, and Peter Domokos. “Observation of the photon-blockade breakdown phase transition.” *Physical Review X* 7, no. 1 (2017): 011012.

[4] Sett, Riya, Farid Hassani, Duc Phan, Shabir Barzanjeh, Andras Vukics, and Johannes M. Fink. “Emergent macroscopic bistability induced by a single superconducting qubit.” *PRX Quantum* 5, no. 1 (2024): 010327.

[5] Domby, András et al. “Collective self-trapping of atoms in a cavity.” *New J. Phys.* 23 (2021): 083036

[6] Gábor, Bence et al. “Ground-state bistability of cold atoms in a cavity.” *Physical Review A* 107.2 (2023): 023713; Gábor, Bence et al. “Quantum bistability in the hyperfine ground state of atoms.” *Physical Review Research* 5.4 (2023): L042038.

Hot Topic Talk, Thursday 18:20-18:40, Saal Tirol

Ultrafast imaging of ytterbium tweezer arrays

Alessandro Muzi Falconi¹; Omar Abdel Karim²; Riccardo Panza³; Riccardo Forti¹; Sara Sbernadori³; Matteo Marinelli¹; Francesco Scazza³

¹ University of Trieste

² CNR-INO, University of Napoli

³ University of Trieste, CNR-INO

Detecting and manipulating individual atoms with high fidelity is essential for quantum simulation, metrology and, with even more stringent requirements, for quantum computing. I will present our recent results on ultrafast single-atom imaging, based on alternated pulses of highly saturated light addressing the broad $1S_0$ - $1P_1$ transition in ytterbium. With this scheme, we achieve in-trap single-atom detection fidelity and survival probability exceeding 99.8% within just few microseconds.

Beyond single-atom detection, we extend this ultrafast imaging scheme to the detection of multiple atoms in free space with single-particle resolution. By preparing and releasing multiply filled traps, we demonstrate single-atom-resolved detection without parity projection. This capability will enable new explorations of correlations and many-body dynamics in tweezer-trapped atomic ensembles.

Finally, I will also mention the newest tweezer-based quantum platform under construction at the University of Trieste. This system integrates three key components: a quantum computing unit for executing arbitrary operations, a tweezer-cavity interface for cavity quantum electrodynamics and quantum networking experiments, and an atom reservoir to enable fast experimental cycle times and uninterrupted operations. This architecture will serve as a versatile testbed for advancing neutral atom quantum technologies.

Collisions 3

Invited Talk, Thursday 17:00-17:30, Saal Straßburg

Quantum resonances in cold collisions

Christiane Koch

Freie Universität Berlin

Quantum resonances in low-energy collisions are a sensitive probe of the intermolecular forces. They dominate the final quantum state distribution even for strong and highly anisotropic interactions, as recently observed for Feshbach resonances populated by Penning ionization of dihydrogen colliding with a metastable rare gas atom [1]. For such a small collision complex, full quantum scattering calculations can be carried out [1]. The theoretical predictions for the cross section involve then only the approximations made when constructing the potential energy surface (PES). Changes in the shape of the PES thus translate directly into modifications of the cross sections. This can be used to improve calculated PES, starting from the experimental data [2]. Conversely, one can also ask by how much the experimental resolution of measured cross sections must improve in order to unambiguously discriminate predictions derived from different levels of advanced ab initio electronic structure theory [3]. Such discrimination is equivalent to resolving the intermediate resonances governing the reaction dynamics, on top of the initial and final states.

[1] Margulis et al., *Science* 380, 77 (2023)

[2] Horn et al., *Science Advances* 10, eadi6462 (2024)

[3] Horn et al., arXiv:2408.13197

Invited Talk, Thursday 17:30-18:00, Saal Straßburg

Cold and controlled collisions using tamed molecular beams

Bas van de Meerakker

Radboud Universiteit, Nijmegen

The study of molecular collisions with the highest possible detail has been an important research theme in physical chemistry for decades. Experimentally, the level of detail obtained in these studies depends on the quality of preparation of the collision partners before the collision, and on how accurately the products are analyzed afterward.

Over the last years, methods have been developed to get improved control over molecules in a molecular beam. With the Stark decelerator, a part of a molecular beam can be selected to produce bunches of molecules with a computer-controlled velocity and with longitudinal temperatures as low as a few mK. The molecular packets that emerge from the decelerator have small spatial and angular spreads, and have almost perfect quantum state purity. These tamed molecular beams

are excellent starting points for high-resolution crossed beam scattering experiments.

I will illustrate the possibilities this new technology offers to study molecular collisions with unprecedented precision and at low collision energies. I will discuss our most recent results on the combination of Stark deceleration and velocity map imaging. The narrow velocity spread of Stark-decelerated beams results in scattering images with an unprecedented sharpness and angular resolution. This has facilitated the observation several quantum effects in state-to-state cross sections, such as diffraction, scattering resonances and product pair correlations in bimolecular collisions. Finally, I will present recent results on bimolecular collisions at collision energies down to 0.1 cm⁻¹ obtained by merged beam configurations, featuring novel effects induced by the dipole-dipole interaction.

Hot Topic Talk, Thursday 18:00-18:20, Saal Straßburg

Electron Diffraction Imaging of Molecules via Ionization by Compton Scattering

A. Kügler¹; A. Pier¹; D. M. Haubenreißer²; F. Trinter³; I. Dwojak¹; J. Drnec⁴; J. Kruse¹; J. Stindl¹; L. Kaiser¹; L. Nowak¹; L. Ph. H. Schmidt¹; L. Sommerlad¹; M. Kircher¹; M. S. Schöffler¹; M. Schmidt¹; N. Anders¹; N. M. Novikovskiy²; N. Melzer¹; O. D. McGinnis¹; Philipp Demekhin²; R. Dörner¹; T. Jahnke⁵

¹ Institut für Kernphysik, Goethe-Universität Frankfurt, Germany

² Institut für Physik und CINSaT, Universität Kassel, Germany

³ Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

⁴ ESRF, The European Synchrotron, Grenoble Cedex 9, France

⁵ Max-Planck-Institut für Kernphysik, Heidelberg, Germany; European XFEL, Schenefeld, Germany

Compton scattering is the fundamental light-matter interaction process discussed in the textbooks as a billiard-type collision, in which a photon (as a particle) is deflected and transfers parts of its energy and momentum to an electron initially at rest. If electron is bound in an atom or molecule, its momentum distribution contributes to the balance, which is known as the impulse approximation [1]. As a consequence, the momentum distribution of direct Compton electrons is given by the Fourier transform of the initial orbital displaced by the photon momentum transfer. Recent experimental and theoretical studies [2,3] highlighted the need to go beyond this approximation. In particular, Ref. [2] reported a backward scattering of the direct Compton electrons with respect to the photon momentum transfer and a simultaneous forward kick of the parent nucleus, while Ref. [3] demonstrated a scattering of the direct Compton electrons to all angles and a Coulomb focusing of the electrons by the ionization potential of the ion.

In the present work, we consider theoretically and experimentally the K-shell ionization of C and O atoms in carbon monoxide molecules by Compton scattering of 20 keV photons and report differential electron momentum distributions [4]. We observe diffraction patterns in the momentum distributions, which persist after integration over magnitudes and orientations of the photon momentum transfer in the frame of molecular reference. This phenomenon relies on the interference of the direct Compton electrons and those which are scattered on the parent and neighboring nuclei. The double-slit interference patterns in the electron momentum distribution can directly be related to the molecular orientation and the internuclear distance. The present results suggest that the imaging techniques, widely employed in the optical regime via laser-induced diffraction and soft x-ray domain via one-photon inner-shell photoionization, can be extended to the hard X-ray domain, where the photoionization is strongly suppressed, and the ionization by Compton scattering became dominant.

- [1] J. W. M. Du Mond, Phys. Rev. 33, 643 (1929).
- [2] M. Kircher et al., Nat. Phys. 16, 756 (2020).
- [3] N. Melzer et al., Phys. Rev. Lett. 133, 183002 (2024).
- [4] D. M. Haubenreißer et al, (2025) submitted

Hot Topic Talk, Thursday 18:20-18:40, Saal Straßburg

Convergent Close-Coupling Approach to Electron-Impact Dissociative Excitation and Ionisation of H₃⁺

Reese Horton¹; Michael Pak²; Igor Bray¹; Dmitry Fursa¹

¹ Curtin University

² Air Force Institute of Technology

The results of a newly developed version of the Molecular Convergent Close-Coupling (MCCC) method [1,2] of calculating cross sections for electron scattering on the H₃⁺ molecule are reported. Integrated cross sections for dissociative electronic excitation and ionisation are presented, yielding good agreement with the experiment [3,4]. The causes of previous disagreements between theory and experiment are identified. The method is presented in both the fixed-nuclei and adiabatic nuclei formulations, with optional point-group symmetry adaptation. The results of the first-ever calculation of fragment kinetic energy release distributions in electron impact dissociation of H₃⁺ are also reported, yielding good agreement with the strong textexperiment at high energies. The new method opens the door to the modelling of electron and positron scattering on polyatomic molecules using CCC techniques.

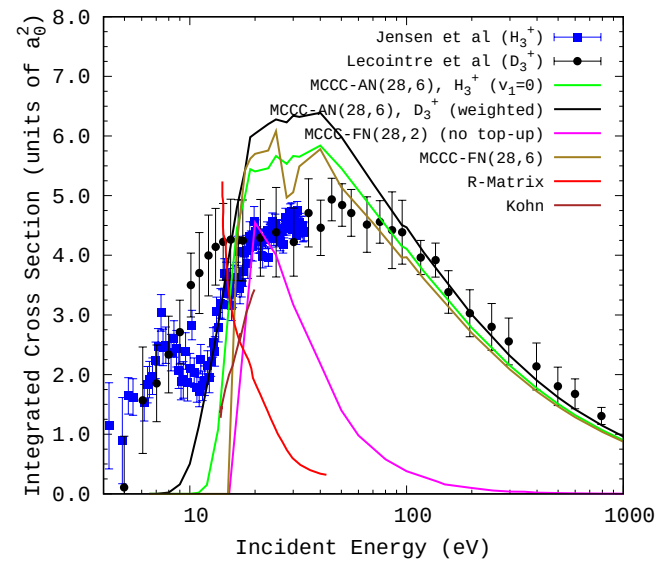


Fig.: Comparison of the total dissociative excitation cross section for electron scattering on H₃⁺ and D₃⁺ in several MCCC models [1,2] with the experiments of Lecointre et al [3], Jensen et al [4], the R-matrix calculation of Gorfinkel and Tennyson [5] and the complex-Kohn calculation of Orel [6].

- [1] Horton et al, Phys. Rev. Lett. 134, 063001 (2025).
- [2] Horton et al, Phys. Rev. A. 111, 022802 (2025).
- [3] Lecointre et al, J. Phys. B. 42, 075201 (2009).
- [4] Jensen et al, Phys. Rev. A. 63, 052701 (2001).
- [5] Gorfinkel and Tennyson, J. Phys. B 38, 1607 (2005).
- [6] Orel, Phys. Rev. A. 46, 1333 (1992).

Quantum 4

Invited Talk, Friday 10:30-11:00, Saal Brüssel

Many-body theory and calculations of positron binding, scattering and annihilation in polyatomic molecules

Dermot Green

Queen's University Belfast

Positrons are unique probes of matter, with applications in materials science (ultra-sensitive diagnostic studies of surfaces, defects and porosity), medical imaging (positron emission tomography), astrophysics, molecular spectroscopy, and are central to the formation of more complicated antimatter, including positronium and antihydrogen, used for studies of fundamental physics.

Low-energy positron interactions with atoms and molecules are characterized by strong many-body correlations, including positron-induced polarization of the molecular electron cloud, screening of the electron-positron Coulomb interaction, and the unique process of virtual-positronium formation (where a molecular electron temporarily tunnels to the positron). They enhance annihilation rates by orders of magnitudes, modify scattering cross sections and annihilation γ spectra, and can enable positron binding. They also make the description of positron-atom/molecule interactions –required to properly interpret fundamental experiments and materials science techniques, and develop antimatter-based technologies– a challenging theoretical and computational problem.

I will present our recently developed *ab initio* many-body theory description of positron binding, scattering and annihilation in polyatomic molecules, and its state-of-the-art computational implementation in our open-source EXCITON+ code [1]. Since early 2000's, positron binding energies had been measured for around ~100 molecules. However, accurate *ab initio* calculations had proved elusive, with previous sophisticated quantum chemistry calculations severely deficient, giving agreement to at best 25% error (see [1] and references therein). By properly accounting for the correlations, our many-body theory approach has provided the first *ab initio* description of positron binding to molecules in agreement with experiment (see e.g., [1-3]). It has also provided fundamental insight into the role of correlations and molecular symmetry and predicted binding energies in other molecules including nucleobases [1-3]. Its predictive capability has also been demonstrated via joint theory-experimental work in which binding energies for ringed hydrocarbons were calculated in agreement with new measurements [3]. In addition, it has predicted new classes of positronically-bonded molecules (where two otherwise repulsive anionic species are stabilized by a positronic bond) [4]. I will also discuss recent developments extending the method and EXCITON+ code to enable *ab initio* calculation of positron scattering [5] and annihilation γ -ray spectra on polyatomic molecules [6].

This work was/is supported by the European Research Council grants 804383 & 101170577. It was performed with J. Hofierka, B. Cunningham, C. Rawlins, J. Cassidy, S. Gregg and A. Swann, and in collaboration with Charles Patterson (TCD) and the UCSD experimental positron group of Cliff Surko & James Danielson and colleagues.

- [1] J. Hofierka, ..., D.G. Green, *Nature* 606, 688 (2022).
- [2] J. Cassidy, ..., D.G. Green, *PRA Letter* 109, L040801 (2024).
- [3] A. Baidoo, ..., D.G. Green, *PRA* 109, 062801 (2024).
- [4] J. Cassidy, ..., D.G. Green, *JCP (Spec.-Collec.)* 160, 084304 (2024).
- [5] C. M. Rawlins, ..., D.G. Green, *PRL* 130, 263001 (2023), & in prep.-(2025).
- [6] S. K. Gregg, ..., D.G. Green, *arXiv:2502.12364* (2025).

Invited Talk, Friday 11:00-11:30, Saal Brüssel

Quantum Optics with Rydberg Excitons

Alistair Brewin¹; Jonathan Pritchett²; Horatio Wong¹; Madeleine Fisher¹; Liam Gallagher¹; C. Stuart Adams¹; Kieran O'Brien¹; Robert Potvliege¹; Stewart Clark¹; Matthew Jones¹; Stephen Lynch³; Wolfgang Langbein³; Simon Doyle³

¹ Durham University

² King's College London

³ Cardiff University

Quantum optics with Rydberg atoms and superconducting resonators is well-established, with attention now towards interfaces with on-chip quantum computing devices [1,2]. We are developing a similar platform using Rydberg excitons –bound states of excitons and holes in a semiconductor. We have measured the largest microwave-optical Kerr coefficient to date [3], and our experiments are able to reach the ultra-strong driving limit where the coupling strength exceeds the splitting between nearby Rydberg states [4]. These results are in near-quantitative agreement with an atomic-physics inspired theoretical models [3,4]. Rydberg excitons may also exhibit optical strong coupling [5], and I will describe our progress towards a hybrid quantum system of Rydberg excitons strongly coupled to on-chip optical and microwave resonators at T<300 mK.

- [1] A. A. Morgan and S. Hogan, *Phys. Rev. Lett.* 124, 193604 (2020)
- [2] M. Kaiser et al., *Phys. Rev. Res.* 4, 013207 (2022)
- [3] J. D. Pritchett et al. *APL Photonics* 9, 031303 (2024)
- [4] A. Brewin et al., *New J. Phys.* 26, 113018
- [5] K. Orfanakis et al., *Nature Materials* 21, 767 (2022).

Invited Talk, Friday 11:30-12:00, Saal Brüssel

Adiabatic echo protocols for robust quantum many-body state preparation

Hannes Pichler

IQOQI & University of Innsbruck

Entangled many-body states serve as foundational resources for advancing quantum technologies. However, reliably preparing these states in interacting quantum systems often faces significant challenges due to unavoidable experimental imperfections. In this talk, I will introduce the “adiabatic echo protocol,” a novel and general method designed to robustly prepare many-body entangled states by dynamically suppressing the effects of static perturbations.

I will explain the underlying principle of dynamically engineered destructive interference that underpins its robustness and demonstrate how this protocol emerges naturally through quantum optimal control techniques, without restrictive assumptions on the form of the control fields. Practical examples from our research include the preparation of Greenberger-Horne-Zeilinger (GHZ) states in ferromagnetic Ising chains, two-dimensional Rydberg atom arrays, and quantum spin liquid states in frustrated Rydberg lattices.

Our findings emphasize the versatility and broad applicability of the adiabatic echo protocol, presenting a viable approach for dependable many-body state preparation within current quantum experimental platforms

Hot Topic Talk, Friday 12:00-12:20, Saal Brüssel

From Quantum Statistics to Work: The Pauli Engine and Beyond

Keerthy Menon¹; Thomas Fogarty¹; Eloisa Cuestas²;
Jennifer Koch³; Sian Barbosa³; Eric Lutz⁴; Artur Widera³;
Thomas Busch¹

¹ OIST Graduate University

² Forschungszentrum Jülich

³ RPTU Kaiserslautern-Landau

⁴ University of Stuttgart

Heat engines convert thermal energy into mechanical work and have been extensively studied in the classical and quantum regimes. In the quantum domain, however, nonclassical forms of energy exist, which are distinct from traditional heat and which can also be harnessed to generate work in cyclic engine protocols.

We introduce the concept of the Pauli engine: a novel quantum many-body engine powered by the energy difference between fermionic and bosonic ultracold particle ensembles, arising from the Pauli exclusion principle. The distinct quantum statistics lead to a redistribution of population across energy levels, enabling engine cycles that replace traditional heat strokes in the quantum Otto cycle. This concept has recently been realized experimentally in the BEC-BCS crossover regime [1].

Building on this idea, we also present several concepts for hybrid quantum-classical engines, where a change in quantum statistics is implemented either during the adiabatic work strokes or the isochoric heat strokes. While the Pauli engine alone demonstrated high efficiency, we show that combining quantum and classical effects can further enhance both efficiency and work output. All cycles are discussed in the context of ultracold atomic gases, which are well suited for their experimental realisation.

[1] J. Koch, K. Menon, E. Cuestas, S. Barbosa, E. Lutz, T. Fogarty, Th. Busch, A. Widera, *Nature* 621, 723 (2023).

Hot Topic Talk, Friday 12:20-12:40, Saal Brüssel

Quantum-enabled Rydberg atomic polarimetry of radio-frequency fields

Matthew Cloutman¹; Matthew Chilcott¹; Alexander Elliott²; Susanne Otto¹; Amita Deb³; Niels Kjærgaard¹

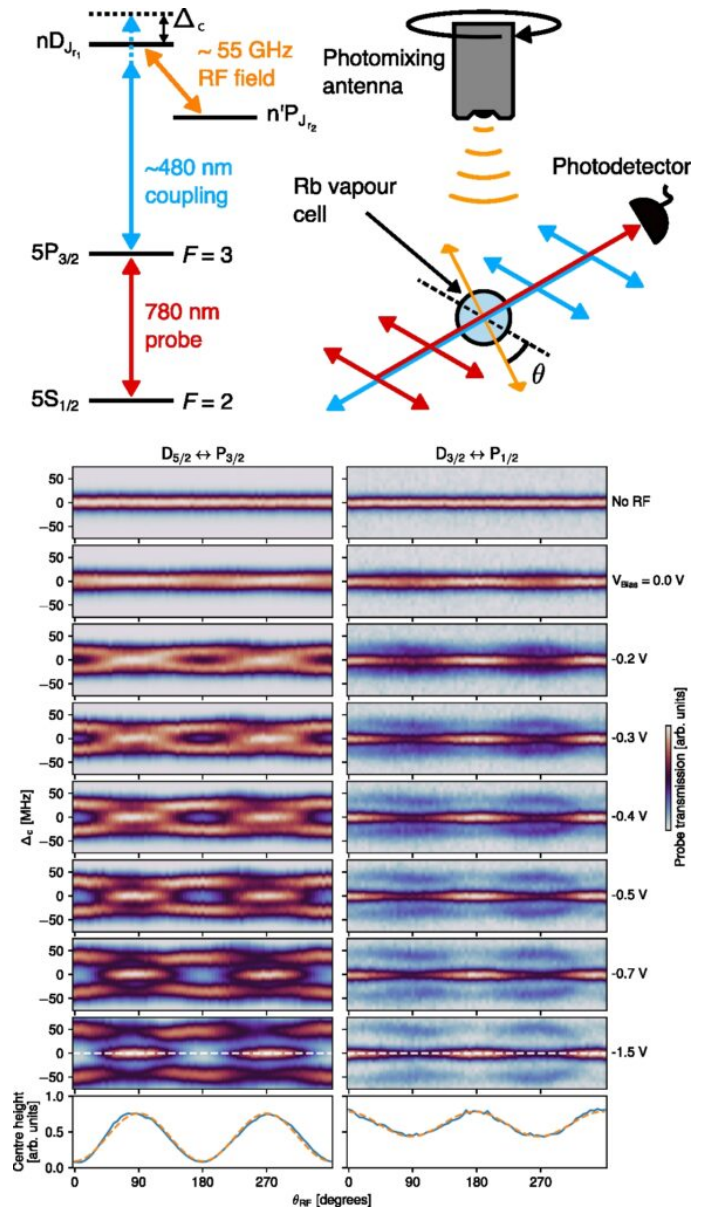
¹ Department of Physics, University of Otago, and Dodd-Walls Centre for Photonic and Quantum Technology, Dunedin, New Zealand

² Department of Physics, University of Auckland and Dodd-Walls Centre for Photonic and Quantum Technology, New Zealand

³ School of Physics and Astronomy, University of Birmingham, United Kingdom

Rydberg atoms efficiently links photons between the radio-frequency (RF) and optical domains. They provide a medium in which the presence of an RF field imprints on the transmission of a probe laser beam by altering the coherent coupling between atomic quantum states. The immutable quantized energy structure of the atoms underpins quantum-metrological RF field measurements and has driven intensive efforts to realize inherently self-calibrated sensing devices. Here we investigate spectroscopic signatures owing to angular momentum quantisation of the atomic states utilized in an electromagnetically-induced transparency (EIT) sensing scheme. Specific combinations of atomic terms are shown to give rise to distinctive fingerprints in the detected optical fields upon rotating the

RF field polarization.



The characteristic angular variation for a term combination is universal and independent of the atomic species involved. By examining two ostensibly similar angular momentum ladders, we unveil a striking complementarity in their spectroscopic responses. Our study adds an important new building block for quantum metrological electric field characterisation via Rydberg atomic polarimetry.

Fundamental 2

Invited Talk, Friday 10:30-11:00, Saal Tirol

Nuclear-solid interactions in Thorium-229

Thorsten Schumm; Adrian Leitner; Fabian Schaden;
Georgy Kazakov; Ira Morawetz; Kjeld Beeks; Luca
Toscani de Col; Thomas Riebner; Tomas Sikorsky

TU Wien

Several recent experiments performing VUV laser nuclear spectroscopy of Thorium-229 doped into calcium fluoride single crystals allow to probe nuclear properties and host material parameters with unprecedented accuracy. In this talk I will resume our current understanding of the microscopic doping structure, combining theoretical modelling, solid-state techniques like XAFS and RBS, and precision laser spectroscopy. We also report quenching of the thorium-229 isomer population under X-ray and laser illumination in the VUV, UV and optical range, indicating a strong and controllable coupling of nuclear and solid-state degrees of freedom.

Invited Talk, Friday 11:00-11:30, Saal Tirol

Testing quantum electrodynamics in extreme fields using helium-like uranium

R. Loetzsch¹; H. F. Beyer²; Louis Duval³; U. Spilmann²;
D. Banas⁴; Perla Dergham⁵; F. M. Kröger⁶; Jan Glorius²;
R. Grisenti²; M. Guerra⁷; A. Gumberidze²; R. Hess²;
Pierre-Michele Hillenbrand⁸; P. Indelicato⁹; P.
Jagodzinsk⁴; Emily Lamour⁵; B. Lorentz²; S. Litvinov²; Y.
A. Litvinov²; J. Machado⁷; N. Paul¹⁰; G. G. Paulus⁶; N.
Petridis²; J. P. Santos⁷; M. Scheidel²; R.S. Sidhu²; M.
Steck²; Sébastien Steydl⁵; K. Szary⁴; S. Trotsenko²; I.
Uschmann¹¹; G. Weber²; T. Stöhlker²;

Martino Trassinelli¹²

¹ Helmholtz-Institut Jena

² GSI Helmholtzzentrum für Schwerionenforschung

³ Institut des NanoSciences de Paris, CNRS and Sorbonne University and Laboratoire Kastler Brossel, CNRS, ENS-PSL, Collège de France, Sorbonne Université

⁴ Institute of Physics, Jan Kochanowski University

⁵ Institut des NanoSciences de Paris, CNRS and Sorbonne University

⁶ Helmholtz-Institut Jena, Jena, Germany

⁷ Laboratory of Instrumentation, Biomedical Engineering and Radiation Physics, NOVA University

⁸ Justus-Liebig-Universität Gießen

⁹ Laboratoire Kastler Brossel, Sorbonne Université, ENS-PSL, Collège de France, CNRS

¹⁰ Laboratoire Kastler Brossel, Sorbonne Université, ENS-PSL, Collège de France, CNRS

¹¹ Institut für Optik und Quantenelektronik, Friedrich-Schiller-Universität

¹² CNRS, Institut des NanoSciences

Transition energy measurements in heavy, few-electron ions are unique tools to test bound-state quantum electrodynamics (QED) in extremely high Coulomb fields, where perturbative methods cannot be implemented. In such fields, the effects of the quantum vacuum fluctuations on the atomic energies are enhanced by several orders of

magnitude with respect to light atoms. However, up to now, experiments have been unable to achieve sensitivity to higher-order (two-loop) QED effects in this strong regime. Here we present a novel multi-reference method based on Doppler-tuned x-ray emission from fast uranium ions stored in the ESR ring of the GSI/FAIR facility. By accurately measuring the relative energies between $2p_{3/2} \rightarrow 2s_{1/2}$ transitions in two-, three-, and four-electron uranium ions, we were able, for the first time in this regime, to disentangle and test separately high-order (two-loop) one-electron and two-electron QED effects, and set a new important benchmark for this theory in the strong field domain [1]. The achieved accuracy of 37 parts per million allows us to discriminate between different theoretical approaches developed throughout the last decades for describing He-like systems. Experimental outlooks will be presented, as new calibration schemes and the implementation of a new time- and position-sensitive detector, based on Timepix3 technology. These considered improvements will allow for a reduction of the uncertainties by another order of magnitude, lower than the present theoretical prediction uncertainties and nuclear deformation effects.

[1] R. Loetzsch *et al.*, Nature **625**, 673-678 (2024).

Hot Topic Talk, Friday 11:30-11:50, Saal Tirol

Vortices in a dipolar supersolid and single erbium atoms in optical tweezers

Manfred Mark; Eva Casotti; Elena Poli; Clemens Ulm;
Lauritz Nathanael Klaus; Andrea Litvinov; Daniel
Schneider Grün; Riccardo Donofrio; Arina Tashchilina;
Francesca Ferlaino

Institut für Experimentalphysik, Universität Innsbruck

Supersolids are exotic states of matter that spontaneously break two symmetries: gauge invariance through the phase-locking of the wavefunction, and translational symmetry owing to the emergence of a crystalline structure. In a first part, we report on the theoretical study and experimental observation of vortices in a dipolar supersolid of Dysprosium [1]. When rotated, the supersolid phase shows a mixture of rigid-body and irrotational behavior, highlighting a fundamental difference between modulated and unmodulated superfluids.

Neutral atoms in optical tweezers are one of the most promising platforms for quantum simulation and computation as they offer the implementation of arbitrary geometries, dynamical reconfiguration, generation of free-defects arrays and controllable long-range coupling via Rydberg-mediated interactions. In the second part, we will present our latest results on the successful loading and detection of single erbium atoms in a linear array of optical tweezers [2]. By implementing two complementary techniques for single atoms detection - narrow-linewidth non-destructive and broad-linewidth ultrafast imaging - we characterized the differential light shift for the intercombination line of erbium, and we investigated light-assisted collisions (LAC) and heating-induced losses.

[1] Observation of vortices in a dipolar supersolid, E. Casotti, E. Poli, L. Klaus, A. Litvinov, C. Ulm, C. Politi, M. J. Mark, T. Bland, F. Ferlaino, Nature, 635, 327-331, 2024

[2] Optical Tweezer Arrays of Erbium Atoms, D. S. Grun, S. J. M. White, A. Ortu, A. Di Carli, H. Edri, M. Lepers, M. J. Mark, F. Ferlaino, Phys. Rev. Lett., 133, 223402, 2024

Hot Topic Talk, Friday 11:50-12:10, Saal Tirol

Collective effects in thermometry and cooling of trapped ions

Ivan Vybornyi; Klemens Hammerer

Leibniz University Hannover

Crystals of cold trapped ions are a promising platform for quantum technology and for studying the quantum many-body problem as a well-controlled toy many-body system. In modern state-of-the-art experiments, managing the entropy of large Coulomb crystals becomes challenging due to the exponential scaling of the Hilbert space with the number of trapped ions. In particular, as we demonstrate, collective effects must be taken into account and play an important role in both motional temperature measurement and the cooling process. Regarding the latter, the possible influence of collective effects has been debated in the literature in recent years. In my talk, I will present a thermometry protocol for large ion crystals that accounts for the emerging collective dynamics [1] and describe a mechanism that enhances the cooling of collective modes as more ions are added to the crystal.

[1] I.Vybornyi et. al, PRX Quantum 4, 040346 (2023)

Ultrafast 4

Invited Talk, Friday 14:00-14:30, Saal Brüssel

Generation of optical Schrödinger "cat" states using intense laser-matter interactions and applications in non-linear optics

Paraskevas Tzallas

FORTH-IESL

Intense laser-matter interaction leads to high harmonic generation (HHG), where the low frequency photons of a driving laser field are converted into photons of higher frequencies. This process has enabled breakthroughs in AMO physics and attosecond science [1]. Until recently, it was described by classical or semi-classical approaches [2], ignoring the quantum nature of light.

Recent investigations conducted using fully quantized approaches have shown how the HHG process can be used for the generation of optical Schrödinger "cat" and entangled light states from the infrared to the extreme-ultraviolet spectral range [3-10].

Here, after a brief introduction, I will focus my talk on the most recent studies concerning the generation of optical "cat" states and their role in nonlinear optics [11]. I will also emphasize the potential of using fully quantum approaches in laser-driven semiconductor crystals to develop non-classical and entangled light states in the VUV spectral region with attosecond pulse duration [12]. Finally, I will briefly discuss some additional representative key approaches developed in the recent past by other groups in this research field [13-19].

References

- [1] P. Agostini, F. Krausz and A. L'Huillier Nobel prize in physics 2023
- [2] K. Amini, et al., Rep. Prog. Phys. 82, 116001 (2019) (and references herein).
- [3] M. Lewenstein, et al., Nat. Phys. 17, 1104 (2021).
- [4] J. Rivera-Dean, et al., Phys. Rev. A 105, 033714 (2022).
- [5] P. Stammer, et al., PRL 128, 123603 (2022).
- [6] J. Rivera-Dean arXiv:2409.02016
- [7] P. Stammer arXiv:2410.15503
- [8] P. Stammer, et al., PRX Quantum 4, 010201 (2023).

- [9] U. Bhattacharya, et al., Rep. Prog. Phys. 86, 094401 (2023).
- [10] J. Rivera-Dean et al., PRB 109, 035203 (2024).
- [11] Th. Lamprou, et al., PRL 134, 013601 (2025).
- [12] A. Nayak et al., Nat. Commun. 16,1428 (2025)
- [13] M. E. Tzur, et al., Nat. Photon. 17, 501 (2023).
- [14] A. Goriach, et al., Nat. Phys. 19, 1689 (2023)
- [15] J. Heimerl, et al., Nat. Phys. 20, 945 (2024).
- [16] D. Theidel, et al., PRX Quantum 5, 040319 (2024).
- [17] S. Lemieux, et al., arXiv:2404.05474 (2024).
- [18] A. Rasputnyi, et al., Nat. Phys. 20, 1960 (2024).
- [19] S. Yi, et al., Phys. Rev. X 15, 011023 (2025).

Invited Talk, Friday 14:30-15:00, Saal Brüssel

Two-dimensional sub-wavelength topological lattices for dark-state ultracold atoms

Gediminas Juzeliūnas; Domantas Burba

Vilnius University

Ultracold atoms represent a flexible platform for simulating topological and many-body phenomena of condensed matter and high-energy physics. The use of atomic dark states (long-lived superpositions of atomic internal ground states immune to atom-light coupling) offers new possibilities for such simulations. Making the dark states position-dependent, one can generate a synthetic magnetic field for ultracold atoms adiabatically following the dark states [1]. Recently, two-dimensional (2D) dark-state lattices were considered [2,3].

Here we present a general description of 2D topological dark state lattices elucidating an interplay with the sub-wavelength lattices [4]. In particular, we demonstrate that one can create a 2D Kronig-Penney lattice representing a periodic set of 2D subwavelength potential peaks affected by a non-staggered magnetic flux. Away from these patches of the strong magnetic field, there is a smooth magnetic flux of the opposite sign, compensating for the former peaks. While the total magnetic flux is zero, the system supports topological phases due to the flux variation over a unit cell, akin to Haldane-type lattice models with zero net flux over an elementary cell, but non-trivial topology due to non-zero fluxes over the plaquettes constituting the elementary cell. This work paves the way for experimental exploration of topological phases in dark-state optical lattices, offering new possibilities for simulating quantum Hall systems, fractional Chern insulators and related strongly correlated phases.

- [1] N. Goldman, G. Juzeliūnas, P. Öhberg, and I. B. Spielman, Rep. Prog. Phys., 77,126401 (2014).
- [2] E. Gvozdiavas, I. B. Spielman, and G. Juzeliūnas, Phys. Rev. A, 107, 033328 (2023).
- [3] S. Nascimbene and J. Dalibard, arXiv:2412.15038 (2024).
- [4] D. Burba and G. Juzeliūnas, to be published.

Hot Topic Talk, Friday 15:00-15:20, Saal Brüssel

Interplay of locally chiral rotational and electronic currents in chiral molecules

Marjan Mirahmadi¹; Alexander G. Löhr¹; Andres F. Ordóñez²; Olga Smirnova¹

¹ Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy

² Imperial College London

Chiral molecules play a vital role in pharmaceuticals, materials science, and agrochemicals, as their mirror-image forms (enantiomers)

can exhibit different biological and chemical properties. Distinguishing between these enantiomers is challenging, driving research into advanced light-matter interaction techniques, including nonlinear methods based on electric dipole interactions, which can enhance chiroptical sensitivity by orders of magnitude and introduce concepts like local chirality [1]. For instance, locally chiral Lissajous figures of synthetic chiral light can generate strong enantio-sensitive signals in high-harmonic generation [2].

Inspired by this, we examine the interplay between two locally chiral structures: the induced polarization vector of chiral electron currents, and the rotational trajectory of a molecule, both driven by locally chiral fields. Using a pump-probe setup, we analyse how the chiral rotational dynamics affect photoionization and photoexcitation, finding signatures of the interferences between chiral motions evolving on different time scales. This analysis has been conducted for both an achiral molecule and a chiral molecule using chiral hydrogenic electronic states [3] as a model of chiral electronic density. We demonstrate that even achiral spherical top molecules can exhibit chiral rotational trajectories in space (analogous to Lissajous figures of synthetic chiral light) under controlled excitation. Furthermore, by exploring the ultrafast enantio-sensitive electronic response in rotating chiral molecules, we identify new efficient enantio-sensitive observables, such as transient absorption and photoelectron circular dichroism of chiral rotors.

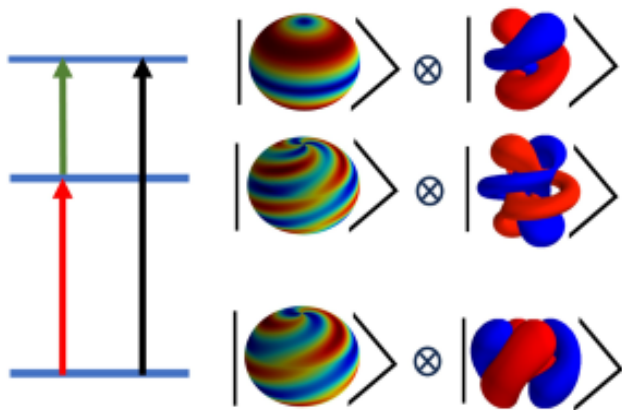


Fig.: Excitation scheme induced by the probe pulse, acting on molecular state as product of chiral rotational wavepacket (left ket in the product) and chiral electronic state (right ket in the product).

Acknowledgement

We gratefully acknowledge ERC-2021-AdG project ULISSES, grant agreement No.101054696

References

- [1] D. Ayuso, A. F. Ordonez, and O. Smirnova, Phys. Chem. Chem. Phys. **24**, 26962 (2022).
- [2] D. Ayuso, *et al*, Nat. Photonics **13**, 866 (2019).
- [3] A. F. Ordonez, and O. Smirnova, Phys. Rev. A **99**, 043416 (2019).

Hot Topic Talk, Friday 15:20-15:40, Saal Brüssel

Femtosecond timed imaging of rotation and vibration of alkali dimers on the surface of helium nanodroplets

Henrik Høj Kristensen¹; Lorenz Kranabetter¹; Areg Ghazaryan²; Nicolaj Jyde¹; Jeppe Christensen¹; Emil Hansen³; Constant Schouder⁴; Frank Jensen¹; Robert Zillich⁵; Mikhail Lemeshko²; Henrik Stapelfeldt¹

¹ Department of Chemistry, Aarhus University

² Institute of Science and Technology Austria

³ Department of Physics, Aarhus University

⁴ ISMO, CNRS, Université Paris-Saclay

⁵ Institute for Theoretical Physics, Johannes Kepler Universität

Alkali dimers, Ak_2 , residing on the surface of helium nanodroplets, are set into rotation and vibration, through the dynamic Stark effect, by a moderately intense 50-fs pump pulse. Coulomb explosion of dimers in the singlet $X^1\Sigma_g^+$ and triplet $a^3\Sigma_u^+$ state [1, 2], induced by an intense, delayed femtosecond probe pulse, is used to record the time-dependent nuclear motion.

Concerning rotation, the measured alignment traces for Na_2 , K_2 , and Rb_2 show distinct periodic features that differs qualitatively from the well-known alignment dynamics of linear molecules in either the gas phase or dissolved in liquid helium [3]. Instead, the observed alignment dynamics of Na_2 and K_2 in the $a^3\Sigma_u^+$ state and of K_2 and Rb_2 in the $X^1\Sigma_g^+$ state agree with that obtained from a 2D rigid rotor model, strongly indicating that the rotation of each dimer occurs in a plane - defined by the He droplet surface [4, 5].

Concerning vibration, the Coulomb explosion probe method enables us to measure the distribution of internuclear distances as a function of time. For K_2 in the $a^3\Sigma_u^+$ state, we observe a distinct oscillatory pattern caused by a two-state vibrational wave packet in the initial electronic state of the dimer. The wave packet is imaged for more than 250 vibrational periods with a precision better than 0.1 Å on its central position. Unlike the rotational motion, the vibration of the dimer is essentially unaffected by the presence of the He droplet [6].

References:

- [1] H. H. Kristensen, et al. Phys. Rev. Lett. **128** (2022), 093201
- [2] H. H. Kristensen, et al. Phys. Rev. A **107** (2023), 023104
- [3] A. S. Chatterley, et al. Phys. Rev. Lett. **125** (2020), 013001
- [4] L. Kranabetter, et al. Phys. Rev. Lett. **131** (2023), 053201
- [5] H. H. Kristensen, et al., In preparation. (Available at arXiv:2502.14521 [physics.atm-clus])
- [6] N. K. Jyde, et al. J. Chem. Phys. **161** (2024), 224301

Spectroscopy 3 / Ultra-cold 4

Invited Talk, Friday 14:00-14:30, Saal Tirol

A pedestrian route to modeling atomic processes

Stephan Fritzsche

HI Jena

Detailed information about atomic excitation and decay processes are

urgently required in many research fields in physics, science and elsewhere, from astro physics to (atomic) spectroscopy and metrology, to the development of light sources, and up to material science, to recall just a few of them [1]. More often than not, this information need to be obtained from atomic computations that are able to provide reliable data on demand. With the Jena Atomic Calculator (JAC), I have developed a relativistic structure code for the computation of atomic amplitudes, properties processed which is suitable for (most) open-shell atoms and ions across the periodic table [2,3].

In this talk, I explain a “pedestrian” route to modeling many, if not most, of these processes [4]. Apart from the frequently employed excitation and (auto-) ionization of atoms and ions, this includes rare processes, such as the collective Auger decay [5] or hyperfine-induced transitions. This route has been found helpful and equally accessible to working spectroscopists, theoreticians as well as code developers.

[1] S. Fritzsche, P. Palmeri and S. Schippers, *Symmetry* 13, 520 (2021)

[2] S. Fritzsche, *Comp. Phys. Commun.* 240, 1 (2019).

[3] <https://github.com/OpenJAC/JAC.jl>

[4] S. Fritzsche et al., *Eur. J. Phys. D* 78, 75 (2024).

[5] Y. Hikosaka and S. Fritzsche, *PRL*, in print (2025).

Invited Talk, Friday 14:30-15:00, Saal Tirol

Liquid-jet photoelectron spectroscopy of aqueous solutions: Electron scattering, electronic structure and work functions

Bernd Winter

Fritz-Haber-Institut, Berlin, Germany

The electronic structure of liquid water and aqueous solutions is directly accessible by liquid-jet photoelectron spectroscopy (LJ-PES). Energies of photoelectron spectral features have so far typically been referenced to the vacuum-energy level, i.e., in relation to the gas phase, which per definition disregards explicit surface properties such as the work function of aqueous solutions. We discuss how the solution work function changes, as a function of solute type and concentration, can be inferred from a LJ-PES measurement, based on an explicit consideration of a solution's Fermi energy. Competing surface-charging effects contributing to energy shifts of solute and solvent spectral features are important to be quantified and will be explored. This inherently connects to the ability to extract accurate electron binding energies from aqueous solution via LJ-PES experiments.

This talk further discusses the application of LJ-PES to provide structural information of biomolecules in a complex aqueous environment, such as adenosine triphosphate interacting with metal cations. This is achieved by the simultaneous analysis of valence, core-level, and non-local autoionization electron signals. We conclude with a consideration on applying electron Velocity Map Imaging (VMI) to liquid jets, with a focus on electron scattering in solution. VMI promises to vastly increase photoelectron collection efficiency and angular range, and in particular to enable the detection of photoelectron angular distributions in a single measurement. This includes the challenging detection of photoelectron circular dichroism (PECD) from aqueous-phase chiral (bio)molecules.

Hot Topic Talk, Friday 15:00-15:20, Saal Tirol

Observation of a new, regular series of highly doubly excited states in Sr

Matthieu G  n  vriez¹; U Eichmann²

¹ Universit   catholique de Louvain

² Max Born Institute

When two electrons are excited far away from the nucleus, their motion results from the subtle balance between electronic repulsion and the Coulomb attraction of the residual ion. The strong electron correlations give rise to complex and fascinating two-electron dynamics that range from chaotic motion to quasi-stable orbits associated with sharp resonances. We report the experimental and theoretical observation of resonances belonging to a new and general type of doubly-excited states with a distinctive two-electron motion. Such states form a regular Rydberg-like series converging to the double-ionization threshold.

Experimentally, ground-state Sr atoms are excited by sequential multiphoton resonant excitation to doubly-excited states of high angular momentum ($L \sim 15$) lying below the $\text{Sr}^+(N = 9 - 15)$ ionization thresholds – less than 0.5 eV below the double-ionization threshold. The excitation spectra reveal the presence of a regular series of lines that persists even at high energy, where most other spectral features merge into an unstructured continuum. To identify the origin of these lines, we combine large-scale theoretical calculations from first principles with simple modelling. The analysis reveals that the states of the series emerge from a surprising binding mechanism: the electronic repulsion creates, through a Stark-like avoided crossing, an effective, adiabatic potential-energy well in which the outermost electron is localized. Such wells appear at each principal quantum number N and give rise to the series, whose properties scale with powers of N that are different from usual Rydberg-state scaling laws. We also discuss the existence of such series in systems other than Sr.

Hot Topic Talk, Friday 15:20-15:40, Saal Tirol

Collisional excitation of interstellar chloronium: accurate rate coefficients with astrophysical applications

S  ndor Demes¹; Alexandre Faure²; Dariusz K  dziera³; Fran  ois Lique⁴

¹ HUN-REN Institute for Nuclear Research

² Universit   Grenoble Alpes - IPAG

³ Nicolaus Copernicus University in Toru  

⁴ Univ Rennes, IPR

Recent astronomical observations [1,2] have shown that chloronium (H_2Cl^+) is an important intermediate in Cl-chemistry of the interstellar medium (ISM) due to its specific thermodynamic properties. For a proper interpretation of the astronomical observations, radiative transfer modelling is required that takes into account the non-local thermodynamic equilibrium (*non-LTE*) effects of the environment through reliable collisional rate coefficients, which have been lacking in the literature so far for chloronium.

We have recently calculated the first accurate 5-dimensional interaction potential between H_2Cl^+ and molecular hydrogen (H_2), which allowed their rotational excitation to be studied from accurate quantum scattering theories [3]. State-to-state rotational (de-)excitation cross sections have been calculated using the numerically exact close-coupling (CC) scattering method for collision energies from the first inelastic threshold up to 1500 cm^{-1} , involving the lowest 21 rotational states for both the ortho and para nuclear spin species. This allowed

the thermal rate coefficients to be derived up to kinetic temperatures of 200 K. Finally, the importance of the collisional rate coefficients is demonstrated by non-LTE radiative transfer modelling of some H_2Cl^+ rotational transitions that have been observed in different interstellar sources.

- [1] D. A. Neufeld *et al.* *Astrophys. J.* 2015, **807**, 54.
- [2] S. H. J. Wallström *et al.* *Astron. Astrophys.* 2019, **629**, A128.
- [3] S. Demes *et al.* *J. Phys. Chem. A* 2025, **129**, 253.

Young Scientist Award

Young Scientist Award Talk, Wednesday 12:00-12:30, Saal Tiro

Advancing cold molecular ion spectroscopy using helium nanodroplets

Elisabeth Gruber

Institute for Ion Physics and Applied Physics, Universität Innsbruck, Technikerstraße 25, 6020 Innsbruck

Helium nanodroplets (HNDs) are highly versatile cryogenic flying nanoreactors that provide a unique environment for the isolation of atomic and molecular ions, as well as the controlled formation of clusters at sub-Kelvin temperatures. Their gentle, ultra-cold nature makes them an ideal platform for spectroscopic studies and for probing physical and chemical processes under well-defined conditions.

In this presentation, I will introduce a novel and efficient method which we have developed for forming helium-tagged molecular ions by using HNDs. These tagged ions are particularly powerful tools for messenger spectroscopy, enabling high-resolution electronic and rovibrational spectroscopy of cold molecular ions with minimal influence from the helium tag [1-3]. I will also highlight recent advances using highly charged HNDs to produce multiply charged molecular ions and discuss their remarkable resilience against Coulomb explosion through efficient cooling within the superfluid environment [4]. In addition, I will outline future directions in which we aim to integrate the HND technique with ion storage devices, opening new pathways for long-term studies of cold ionic species.

References

- [1] S. Bergmeister *et al.*, *Rev. Sci. Instrum.* 94, 055105 (2023)
- [2] S. Bergmeister *et al.*, *Adv. Sci.* 11, 2307816 (2024)
- [3] S. Krasnokutski *et al.*, *Astrophys. J.* 982, 34 (2025)
- [4] L. Ganner *et al.*, *Phys. Rev. Lett.* 133, 023001 (2024)

Poster Session A

#A1: Atomic and molecular spectroscopy, photo-induced processes

Determination of Desorption Energies in Dispersion-dominated Complexes: Role of Nitrogen Substitution and Functional Group

MUHAMMED Shabeeb; Surajit Maity

IIT HYDERABAD

We present the determination of the intermolecular dissociation energies of M-Ar1-3 (Where M= Naphthalene, Naphthol and 2,2 PBI) complexes by measuring the sequential desorption energies of Ar atoms from the aromatic surface. The dispersion-dominated M-Ar1-3 complexes were produced in the gas phase and characterized using resonant two-photon ionization (R2PI) spectroscopy. The disappearance of Franck-Condon active vibrational bands in the R2PI spectrum was utilized to determine the D0(S1) values of dispersively bound molecular complexes. The energy required to desorb a single Ar atom from the Np-Ar, Np-Ar2, and N-Ar3 complexes were bracketed as 522 ± 20 , 522 ± 20 , and 489 ± 53 cm⁻¹, respectively. The corresponding dissociation energies D0(S1) were determined to be 522 ± 20 , 1044 ± 40 , and 1533 ± 93 cm⁻¹, respectively for n=1, 2 and 3. The ground state dissociation energy D0(S0) was calculated by subtracting the Δv shift of the origin band in the excited state D0(S1), and the values were obtained as 507 ± 20 , 1013 ± 40 , and 1489 ± 93 cm⁻¹, respectively, for Np-Ar, Np-Ar2, and Np-Ar3 complexes. The calculated dissociation energies obtained using D4 corrected B3LYP, PBE0 and BH-LYP levels using def2-TZVPP basis set, have shown good agreement with the experimental data, with the best agreement at PBE0 method. The current investigation highlights an effective laser spectroscopic approach to precisely measure the desorption and dissociation energies of non-covalently bound complexes of polycyclic aromatic hydrocarbon molecules.

#A2: Atomic and molecular spectroscopy, photo-induced processes

Airy offset of velocity imaging-based electron spectrometry

Christophe Blondel; Cyril Drag

Centre national de la recherche scientifique

For thirty years, slow electron velocity imaging, a.k.a. SEVI [1], has relied on the idea that the maximum intensity circles obtained when monoenergetic electrons are projected on a detection plane are a direct visualization of transverse velocities. Quantitatively, the squared radii of those circles would directly provide a measure of the electron energy [2].

When the projected electrons emerge from an atomic process, however, they do so as electron waves, so the electron intensity maxima SEVI relies on are no stigmatic images, but the main fringes formed near caustic surfaces. To put it in optical terms, these are electron rainbows and, as Airy observed, "the maximum illumination does not take place at the Geometrical Caustic (...) but (...) on the luminous side of the geometrical position of the rainbow"[3]. Interpreting the radii of the electron rings, classically, as radii proportional to transverse velocities, has thus resulted in a systematic underestimation of the electron energies.

The underestimation does not depend on the energy of the detected electron. It is a constant energy $\Delta = 1.01879... \times \sqrt[3]{(\hbar q F)^2 / (2m)}$,

which, apart from the fundamental constants $\hbar$ (the reduced Planck constant), q (the elementary charge) and m (the electron mass), only depends on the electric field F , in which electron emission has taken place [4]. Numerically, the bias is 18 μ eV in a 380 V/m field, which is the typical order of magnitude of the fields used in SEVI measurements (when not larger ones). Correspondingly, SEVI-measured electron affinities, which are about one third of the electron affinities of reference nowadays, have probably been overestimated by a similar amount. The electron affinities measured by photodetachment microscopy [5], which has always relied on fitting high-resolution electron images with the actual form of the squared electron wave function, are not affected.

- [1] A. Osterwalder, M. J. Nee, J. Zhou & D. M. Neumark, J. Chem. Phys. **121**, 6317 (2004)
- [2] C. Bordas, F. Paulig, H. Helm & D. L. Huestis, Rev. Sci. Instrum. **67**, 2257 (1996)
- [3] G. B. Airy, Trans. Cambridge Philos. Soc. **6**, 379 (1838)
- [4] C. Blondel & C. Drag, Phys. Rev. Lett. **134**, 043001 (2025)
- [5] C. Valli, C. Blondel & C. Delsart, Phys. Rev. A **59**, 3809 (1999)

#A3: Atomic and molecular spectroscopy, photo-induced processes

Light absorption and emission processes involving charge transfer states of weakly-bound molecular ions in noble gas mixture plasmas

Konstantin Kislov; Alexander Narits; Vladimir Lebedev

P.N. Lebedev Physical Institute of the Russian Academy of Sciences

Mixtures of noble gases are regularly present in the active media of high-power gas lasers and in a variety of UV and VUV radiation sources, including excimer lamps and microplasma cell arrays. In addition to atoms and atomic ions, the plasmas of these mixtures contain homonuclear and heteronuclear molecular ions of inert gases. An important feature of heteronuclear BA⁺ ions is the presence of the excited states of the charge transfer character, which dissociate to A + B⁺ configuration. In the plasma of rare gas mixtures the radiative transitions between these states and the low-lying electronic states which dissociate to A⁺ + B system often result in the wide intense band in the visible, UV- and VUV-range, depending on the specific properties of electronic terms of BA⁺ ions both in the initial and final electronic states. In recent years, experimental [1] and theoretical [2,3] studies of such phototransitions have intensified noticeably. The respective emission has been observed in spectra of discharge glow in plasma of inert gas mixtures [4,5], as well as in a plasma of rare gas mixtures excited by ionizing pumping [1]. Studies of the radiative processes involving the charge transfer states of rare gas molecular ions are of an interest for applied problems of diagnostics of high-temperature plasma in fusion reactors [1], as well as development of new sources of wide-band radiation in visible, UV and VUV-ranges.

Despite the wide range of experimental studies of the radiative transitions above, the theoretical studies of these processes are relatively sparse. This is due to the fact that most of the inert gas heteronuclear cations BA⁺ are weakly (like HeXe⁺, NeXe⁺, NeAr⁺) or moderately bound (like ArXe⁺, KrXe⁺, ArKr⁺), and the energies of their first vibrational quantum are usually low. That means that for the correct description of the dynamics of radiative and collisional reactions with these ions it is necessary to take into account all states of the rovibrational quasicontinuum even at room temperatures of the gas component of plasmas. As a result, the theoretical studies of such processes are mostly limited to the case of the lightest heteronuclear ion, HeNe⁺ [2], which has dissociation energy of 647 meV and the vibrational quantum of 131 meV.

We carry out the theoretical study of the light absorption and emission processes involving the charge transfer states of the weakly bound

(NeXe⁺, NeAr⁺) and moderately bound (ArXe⁺, KrXe⁺) rare gas ions. In order to self-consistently treat the contributions from all states of internuclear motion we use an original semiquantal theoretical approach [3,6] based on the quascontinuum approximation for the rovibrational states of the molecular ion both in the initial and final channels of processes. The dynamics of the processes are described on the basis of the theory of the non-adiabatic transitions between the effective electronic terms given by a sum of the electronic terms of BA⁺ ion and the photon energy (if photon is present) in the initial and final channels of the reaction. Four different channels of radiative transitions are considered: photodissociation, photoassociation, bound-bound and free-free transitions. Our approach allows one to treat all these processes uniformly and to perform a comparative quantitative analysis of their efficiencies. We have calculated the contribution of all four channels into the absorption and emission spectra in visible, UV and VUV region in the wide range of parameters of plasma of rare gas mixtures. One of the challenging difficulties in the theoretical study of these processes in weakly bound heteronuclear ions (such as HeXe⁺, NeXe⁺ or NeAr⁺) stems from the fact that potential curves of their final and initial electronic states are almost parallel in the vicinity of equilibrium internuclear distances. Within the frameworks of the standard variants of the theory of non-adiabatic transitions this leads to the presence of the singularities near the maxima of the calculated bands in the emission spectra. Our modified theoretical approach addresses this problem, which allowed us to achieve very good agreement with experimental data on emission spectra of charge transfer photo-processes both for weakly bound (NeXe⁺, NeAr⁺) and moderately bound (ArXe⁺, KrXe⁺) rare gas ions.

References

1. K. Samarkhanov, M. Khasenov, E. Batyrbekov, I. Kenzhina, Y. Sapataev, and V. Bochkov, *Sci. Technol. Nucl. Install.* **2020**, 8891891 (2020).
2. X.J. Liu, Y.Z. Qu, B.J. Xiao, C.H. Liu, Y. Zhou, J.G. Wang, R.J. Buenker, *Phys. Rev. A* **81**, 022717 (2010).
3. A.A. Narits, K.S. Kislov, V.S. Lebedev, *J. Chem. Phys.* **157**, 204307 (2022).
4. Y. Tanaka, K. Yoshino, D. E. Freeman, *J. Chem. Phys.* **62**, 4484, (1975).
5. M. Tsuji, M. Tanaka, Y. Nishimura, *Chem. Phys. Lett.* **262**, 349 (1996).
6. A. Narits, K. Kislov, V. Lebedev, *Atoms* **11**, 60, (2023).

#A4: Atomic and molecular spectroscopy, photo-induced processes

Electron transfer processes and the formation of solvated dielectrons by UV excitation in sodium-ammonia clusters

Sebastian Hartweg

University of Freiburg

Solvated electrons play important roles in the origin and formation of radiation damage in biological tissue as well as for large-scale chemical synthesis, where they are used as strong reducing agents. While in the former case solvated electrons are created by the interaction of liquids with ionizing radiation, in the latter case they are typically produced by the dissolution of alkali metals in liquid ammonia. These sodium ammonia solutions with their many peculiar concentration dependent properties[1,2] are not well understood on a molecular level, despite the many studies conducted on them[1-4]. Molecular clusters of ammonia doped with sodium atoms can serve as useful model systems, enabling the use of gas phase photoelectron and photoion spectroscopic techniques[4-7].

I will present our recent photoelectron photoion coincidence study of small mixed sodium ammonia clusters[7] in which we could, with support from quantum chemical calculations, identify different electron transfer processes occurring after excitation with UV and VUV

radiation. Among these processes, the formation of transient solvated dielectrons and their subsequent decay via an electron-transfer mediated decay process constitutes a direct observation of solvated dielectrons and an intriguing source of low-energy electrons. In a second part I will discuss preliminary results from a time-resolved photoelectron spectroscopy study on large sodium-doped ammonia clusters performed at the LDM endstation of the free electron Laser Fermi, indicating the presence of additional autoionization pathways following the XUV ionization of these clusters.

- [1] Zurek, E., P.P. Edwards, and R. Hoffmann. *Angew. Chem. Int. Ed.*, 2009. 48(44)
- [2] Buttersack, T., P.E. Mason, R.S. McMullen, et al. *Science*, 2020. 368(6495)
- [3] Vöhringer, P. *Annu. Rev. Phys. Chem.*, 2015. 66(1)
- [4] Hartweg, S., A.H.C. West, B.L. Yoder, et al. *Angew. Chem. Int. Ed.*, 2016. 55(40)
- [5] Zeuch, T. and U. Buck. *Chem. Phys. Lett.*, 2013. 579
- [6] West, A.H.C., B.L. Yoder, D. Luckhaus, et al. *J. Phys. Chem. Lett.*, 2015. 6(8)
- [7] Hartweg, S., J. Barnes, B.L. Yoder, et al. *Science*, 2023. 380(6650)

#A5: Atomic and molecular spectroscopy, photo-induced processes

Photoabsorption Spectroscopy using adQTB Dynamics

Etienne Mangaud; Mukul Dhiman

MSME University Gustav Eiffel, Paris

In the following work I will present the spectral properties of acrolein in gas phase and in water studied using adaptive Quantum Thermal Bath (adQTB) method. In this work we show using this method we can possibly recover some of the peaks missed in simple molecular dynamics model and also the broadening of the spectrum. Though QTB and Wigner type methods give some broadening, they are not in good agreement with the experimental observations.

#A6: Atomic and molecular spectroscopy, photo-induced processes

Single Photoionization of vinylcyanoacetylene and methacrylonitrile in Astrophysical Objects

Martin Schwell¹; Bruno Madebène²; Emilie-Laure Zins²; Helgi Rafn Hrodmarsson¹; Jean-Claude Guillemin³

¹ CNRS, LISA UMR 7583, Université Paris-Est Créteil & Université Paris Cité

² CNRS, MONARIS UMR 8233, Sorbonne Université

³ CNRS, ISCR UMR 6226, Université de Rennes

In recent years, the detection rate of molecules in the interstellar medium (ISM) has been accelerating (CDMS 2024) [1]. This is in large part thanks to significant advances in detection techniques and astronomical data processing. Nitriles (or cyanides) are among the most abundant chemical species in the ISM. They are key species in prebiotic chemistry and their role in the so-called RNA world. This simple and reactive functional group offers a unique potential to build up more complex molecules such as ribonucleic acids but also nucleobases. In terms of formation and evolution of these molecules, many physico-chemical processes play an important role, such as desorption from interstellar grains, radiative recombination, photolysis, to

name only a few. In order to estimate the importance of the latter, one must know, for example, absorption cross sections in the UV and VUV spectral domain. The ubiquitous abundance of nitriles might be due to their photostability. In this study we investigate the single photon ionization of two organic nitriles that have been recently detected, namely vinyl cyanoacetylene [2] and methacrylonitrile [3], in the 8 to 15 eV spectral domain. We present ion yield spectra of parent and fragment ions, as well threshold photoelectron spectra. The experiments are completed by quantum-chemical calculations. All results are discussed in the light of the related molecular photodynamics as well as the astrophysical context. Photoionization rates are calculated for typical interstellar radiation fields.

- [1] The Cologne database of Molecular Spectroscopy, cdms.astro.uni-koeln.de
 [2] K.L.K. Lee et al., *Astrophys. J. Lett.* 908, L11, (2021).
 [3] J. Cernicharo et al., *Astron. Astrophys.* 663, L5, (2022).

#A7: Atomic and molecular spectroscopy, photo-induced processes

Photodesorption of CO ices: Rotational and translational energy distributions

Alejandro Rivero Santamaria¹; Antoine Hacquard²; Ferdinand Benoit³; Géraldine Féraud³; Jean-Hugues Fillion³; Jozef Rakovský⁴; Mathieu Bertin³; Maurice Monnerville¹; Romain Basalgète³; Samuel Del Fré¹; Xavier Michaut³

¹ PhLAM

² MONARIS, Sorbonne Université

³ MONARIS

⁴ J. Heyrovský Institute of Physical Chemistry

Photon-stimulated desorption or photodesorption by UV photons is a fundamental process playing a role in interstellar environments and the surface icy satellites in our solar system. Photodesorption has been proposed to provide an efficient non-thermal desorption route of the interstellar ices present in the cold regions of the ISM, contributing to molecular gas phase abundances measured by radio and space telescopes. In the last decade, several photodesorption studies from cold CO condensates have been focused on the experimental determination of UV photodesorption yields using broad band UV sources [1,2]. Complementary studies of these photodesorption yields, using synchrotron radiation, have additionally been able to highlight the first stage of the desorption mechanism, revealing in particular an indirect desorption, induced by an electronic transition (DIET) involving the first electronic excited state of CO $A^1\Pi$ [3] in the 8-10 eV region. We report here more recent pulsed-laser based experiments and ab-initio calculations to fully characterize the desorption mechanism.

This presentation reports on the translational and rovibrational energy of photodesorbed CO molecules from a CO polycrystalline ice ($T = 15$ K) irradiated at ~ 8 eV. The electronic excitation was induced by a pulsed Vacuum-UV (VUV) laser, and the rovibrational states of the photodesorbed CO molecule in their electronic ground state were probed using resonance enhanced multiphoton ionization (REMPI). Pump-probe experiments enable to measure, for the first time, time-of-flights and rotationally resolved spectra providing the kinetic and internal energy distributions of the desorbing particles. Vibrationally cold CO molecules were observed, with rotational and vibrational energy peaking well-below 300 meV [4]. This study is supported by Ab Initio Molecular Dynamics (AIMD) simulations which focused on the description of the vibrational energy redistribution within a 50 CO molecules aggregate [5]. Measured and theoretical energy distributions present both correlation between rotational and translational energy. These studies allow to fully validate the so-called indirect-DIET, triggered by a highly vibrationally excited CO molecule ($v=40$) within the CO cluster.

Références

- [1] K. I. Öberg, G. W. Fuchs, Z. Awad, H. J. Fraser, S. Schlemmer, E. F. Van Dishoeck, and H. Linnartz, "Photodesorption of CO ice," *Astrophys. J.* 662, L23–L26 (2007).
 [2] G. M. Muñoz Caro, A. Jiménez-Escobar, J. Á. Martín-Gago, C. Rogero, C. Atienza, S. Puertas, J. M. Sobrado, and J. Torres-Redondo, "New results on thermal and photodesorption of CO ice using the novel InterStellar Astrochemistry Chamber (ISAC)," *Astron. Astrophys.* 522, A108 (2010).
 [3] E. C. Fayolle, M. Bertin, C. Romanzin, X. Michaut, K. I. Öberg, H. Linnartz, and J.-H. Fillion, "CO ice photodesorption: A wavelength-dependent study," *Astrophys. J.* 739, L36 (2011).
 [4] A. B. Hacquard, R. Basalgète, S. Del Fré, J. Rakovský, A. Rivero Santamaria, F. Benoit, X. Michaut, G. Féraud, M. Bertin, M. Monnerville and J.-H. Fillion, "Photodesorption of CO ices: Rotational and translational energy distributions," *J. Chem. Phys.* 161, 184306 (2024).
 [5] S. Del Fré, A. R. Santamaria, D. Duflot, R. Basalgète, G. Féraud, M. Bertin, J.-H. Fillion, and M. Monnerville, "Mechanism of ultraviolet-induced CO desorption from CO ice: Role of vibrational relaxation highlighted," *Phys. Rev. Lett.* 131, 238001 (2023).

#A8: Atomic and molecular spectroscopy, photo-induced processes

New Spectral Features on Two-Dimensional Optical Spectra arising from Quantum System-Bath Interactions: Implications and Potential Applications

Sachin Prasad¹; Maxim F. Gelin²; Tan Howe-Siang¹

¹ Nanyang Technological University, Singapore

² School of Science, Hangzhou Dianzi University

Two-Dimensional Optical Spectroscopy (2DOS) is a third-order nonlinear optical spectroscopic technique capable of correlating excitations between states in molecular and material systems (1, 2). The technique makes use of three light pulses, two pump pulses and a probe pulse, which when incident on the system generates a third-order signal that can be heterodyne detected by the probe pulse or a local oscillator. In short, the interaction of the system with the first pump pulse generates coherences within the system, which are projected onto a population state by the second pump pulse. Following this, the interaction of the system with the probe pulse generates secondary coherences within the system, whose decay leads to the emission of the signal field. This time-domain signal field is Fourier transformed over the two coherence periods to generate the 2DOS spectrum, where the spectral features on the corresponding spectrum vary over the delay between the pump-pulse pair and probe pulse. This delay, generally known as the waiting time or population time, is scanned to capture dynamic processes within the system of interest.

A 2DOS spectrum comprises of diagonal and off-diagonal cross peak features. Diagonal peaks track individual excited states or transitions, whereas cross peaks relate two individual excited states. These cross peak features are generally assigned to direct bilinear coupling or population transport between states (1, 2). In addition, the lineshapes of the peaks can be analyzed to extract a wealth of information on system-bath interactions. The system-bath interactions can be classical or quantum in nature and dephase the coherences induced by the light fields in the third-order technique. Recently, we reported on the theoretical possibility of a new source of cross peak spectral features which arise on considering quantum system-bath interactions (3).

To theoretically simulate the 2DOS spectra, the system's response to the incident light fields is calculated perturbatively, where the dephasing induced by the system-bath interaction is treated in the interaction picture. Following this, the second-order cumulant approximation is

invoked, where the fluctuation in transition energies of the states are assumed to follow a gaussian distribution (4). This reduces the information on the system-bath interaction to a two-point energy-gap correlation function between the states of the system. The diagonal peaks are described using correlation functions relating a single transition's frequency-gap over a time-interval t , i.e., $C_{ii}(t) = \langle \delta\omega_{ig}(t)\delta\omega_{ig}(0) \rangle$, whereas, cross peaks are described using correlation functions which relate the frequency-gaps of two distinct transitions over the interval t , i.e., $C_{ji}(t) = \langle \delta\omega_{jg}(t)\delta\omega_{ig}(0) \rangle$, where $i \neq j$. In our previous theoretical demonstration (3), we proved that on considering quantum energy-gap cross correlation functions $C_{ji}(t)$, i.e., $C_{ji}(t)$ defined using a quantum mechanical model yielding a complex valued function, such as the Displaced Harmonic Oscillator (DHO), new cross peak spectral features can be observed on the 2DOS spectrum of systems where direct bilinear coupling and population transport between states are absent.

In addition to the new cross peak spectral features, "intra-band coherences" manifest beating features over the waiting time, both along the diagonals and cross peaks of the 2DOS spectrum. These features only arise when quantum frequency-gap correlation functions $C_{ji}(t)$ are used. A classical description of $C_{ji}(t)$ would result in zero cross peak contributions and the inter-state coherence beating features would be absent. We analyze these new cross peak spectral and beating features and describe its potential applications in furthering the 2DOS field along with the physical implication of these features.

References

- (1) Mukamel, S. Multidimensional femtosecond correlation spectroscopies of electronic and vibrational excitations. *Ann. Rev. Phys. Chem.* **2000**, *51*, 691–729.
- (2) Fresch, E.; Camargo, F. V.; Shen, Q.; Bellora, C. C.; Pullerits, T.; Engel, G. S.; Cerullo, G.; Collini, E. Two-dimensional electronic spectroscopy. *Nat. Rev. Methods Primers* **2023**, *3*, 84.
- (3) Prasad, S.; Gelin, M. F.; Tan, H.-S. Cross Peaks on Two-Dimensional Optical Spectra Arising from Quantum Cross-Correlation Functions. *J. Phys. Chem. Lett.* **2024**, *15*, 11485–11495.
- (4) Mukamel, S. *Principles of nonlinear optical spectroscopy*; Oxford University Press, 1995.

Schematic summarizing the work to be presented

#A9: Atomic and molecular spectroscopy, photo-induced processes

The survival mechanisms of dipeptides to space environmental conditions

Laura Carlini¹; Paola Bolognesi¹; Francesco Porcelli¹; Giuseppe Mattioli¹; Dario Barreiro-Lage²; Jacopo Chiarinelli¹; M.V. Vinitha¹; Alicja Domaracka³; Sergio Díaz-Tendero⁴; C. Aparecida Pires da Costa³; H. Rorthard³; P. Boduch³; Lorenzo Avaldi⁵

¹ CNR-ISM, Area della Ricerca di Roma 1, Monterotondo Scalo (Roma), Italy

² Leiden Institute of Chemistry, Universiteit Leiden, Netherland

³ Centre de Recherche sur les Ions, les Matériaux et la Photonique, CEA, CNRS, ENSICAEN, Normandie Université, Caen, France

⁴ Universidad Autónoma de Madrid, IAdChem, IFIMAC

⁵ CNR-Istituto di Struttura della Materia

In a series of combined experimental studies and molecular dynamics simulations on linear and cyclic dipeptides in gas phase we identified pathways that may provide effective mechanisms for their survival to temperature variation or exposition to radiation in space [1]. The most intriguing result is that these molecules may either 'protect' themselves turning the linear structure into a cyclic one by the formation of an intramolecular peptide bond or release reactive neutral/charged fragments which may act as seeds to re-form the dipeptide or even longer linear peptide chains. To investigate these mechanisms when

the molecules are embedded in an environment, we studied the irradiation of homogeneous films of selected biomolecules (Alanine, Linear and Cyclo AlaAla, Linear and Cyclo GlyPhe and Cyclo GlyGly) by 12C4+ beams of 0.98 MeV/u at 10, 80 and 300 K using infrared spectroscopy (IR) at the IRRSUD beamline of GANIL (Caen, France). DFT calculations are used to assign the IR spectra, to rule out unstable conformers, and to identify relevant features for further analysis.

The most interesting results obtained are:

- the apparent destruction cross section indicates that at room temperature the cyclo species are more resistant than the linear ones and the radioresistance of both species is not affected by the temperature in the studied range;
- the variation of the intensity of IR bands as a function of the ion fluence for both Alanine aminoacid and linear AlaAla dipeptide depends on the selected band. In the case of Alanine the observation of a high similarity between the experimental spectra of monomeric alanine after irradiation and linear AlaAla before irradiation lead to the hypothesis that under irradiation alanine undergoes a "polymerization", thus forming a linear dipeptide. Similarly the variation of the IR spectra of the linear AlaAla has been attributed to the elongation of the linear chain leading to the formation of a linear AlaAlaAlaAla by comparison with simulations.

Acknowledgement. COST action CA20129 - Multiscale Irradiation and Chemistry Driven Processes and Related Technologies (MultiChem); Italy-Sweden MARB project (PGR02090) of MAECI; ICSC-Centro Nazionale di Ricerca in High Performance Computing, Big Data and Quantum Computing, funded by European Union-NextGenerationEU (grant CN00000013).

#A10: Atomic and molecular spectroscopy, photo-induced processes

Multiplatform computing of oscillator strengths and transition probabilities in Os V

Patrick Palmeri¹; Alix Niels¹; Exaucé Bokamba Motoumba²; Maxime Brasseur¹; Pascal Quinet¹; Saturnin Enzonga Yoca³

¹ Université de Mons

² Université Marien Ngouabi

³ Conseil Africain et Malgache pour l'Enseignement Supérieur - CAMES

Osmium is the element of the Periodic Table with the atomic number Z equal to

76. In Tokamaks with divertors made of tungsten ($Z = 74$), it will be produced in the neutron-induced transmutation of the latter. Therefore one can expect that their sputtering may generate ionic impurities of all possible charge states in the fusion plasma. As a consequence, these could contribute to radiation losses in these controlled nuclear devices. The knowledge of radiative rates in all the spectra of osmium is thus important in this field. In this framework, a multiplatform approach has been used to determine the Os V radiative properties and estimate their accuracy. The transition probabilities and the oscillator strengths have been computed for the 2677 electric dipole (E1) transitions falling in the spectral range from 400 to 12000 Angstroms. Three independent atomic structure models have been considered; one based on the fully relativistic ab initio multiconfiguration Dirac-Hartree-Fock (MCDHF) method and two based on the semi-empirical pseudo-relativistic Hartree-Fock (HFR) method.

#A11: Atomic and molecular spectroscopy, photo-induced processes

Bayesian methods for quantum logic spectroscopy

Andrea Turci; Brandon Furey; Elyas Mattivi; Mariano Isaza Monsalve; Miriam Kautzky; Philipp Schindler; Rene Nardi; Zhenlin Wu

University of Innsbruck

Quantum control of a wide class of molecules is crucial for advancing a variety of quantum applications. The potential of polyatomic molecular ions in this context can be significantly enhanced using the toolbox provided by quantum information processing and quantum logic spectroscopy (QLS).

These techniques rely on the ability to determine the state of the molecule which is almost impossible to track in some molecular species, such as the CaOH^+ molecule, where the presence of numerous states, closely spaced energy levels, and overlapping transitions make direct state readout difficult.

Quantum logic spectroscopy enables precise interrogation of molecular states by leveraging co-trapped atomic ions. We explore Bayesian state estimation to infer the molecular state distribution based on measurement outcomes, incorporating prior knowledge from the state distribution of the molecule.

To enhance the efficiency of state identification, we implement Bayesian adaptive design, where the next measurement is selected to maximize the expected information gain. In addition, we will compare our simulations with experimental data, refining our understanding of dynamics of the molecular rotation under QLS protocols. Bayesian adaptive design comes with a considerable computational cost but can be made more efficient by the application of deep experiment design, training a neural network to simulate experimental outcomes and optimize measurement strategies. This approach will allow us to make real-time decisions during spectroscopy experiments, dynamically adjusting measurement choices for optimal information extraction.

#A12: Atomic and molecular spectroscopy, photo-induced processes

Structural Characterization of Interstellar Water Ice Analogues: Optical and Morphological Evolution with Deposition Conditions

Delfina Toulouse¹; Xavier Michaut²; Mathieu Bertin²; Jean-Hugues Fillion²; Guilherme Carvalho³; Géraldine Féraud²; Lionel Amiaud⁴

¹ MONARIS, Sorbonne Université

² MONARIS

³ Sorbonne Université

⁴ ISMO, université Paris Saclay

The structure and morphology of interstellar water ice analogues play a crucial role in molecular adsorption and surface chemistry, influencing processes such as H_2 adsorption in cold astrophysical environments. In this study, we investigate the physical properties of amorphous solid water (ASW) ices deposited at 10 K under ultra-high vacuum using the COSPINU2 setup. Employing a multi-probe approach—combining near- and mid-infrared FTIR spectroscopy, He-Ne laser reflectometry, and optical imaging (Hg vapor lamp and white light)—we characterized ASW films grown via background deposition with

thickness ranging from 0 to 5 μm , and at three different deposition rates.

We retrieved the optical constants of the ice films under each condition, finding lower values compared to those reported in the literature [1],[2]. Notably, for higher deposition rates, we observed an abrupt decrease in specular reflectance and increased diffuse scattering, suggesting a phase transition in the ice structure not seen at lower rates. This points toward a restructuring process during deposition, with slower rates favouring the formation of more stable morphologies.

These findings offer critical insight into the microphysical properties of water ice relevant to astrophysical environments. A better understanding of how deposition conditions influence porosity and surface structure will improve models of H_2 adsorption and desorption dynamics. This structural perspective directly supports ongoing efforts to characterize the interaction of HD, H_2 and D_2 with ASW ices and their role in spin-state chemistry and energy transfer mechanisms in cold molecular clouds.

[1] Rebecca A. Carmack et al, 2023, ApJ 942 1

[2] Emily H. Mitchell et al, 2017, Icarus 285

#A13: Atomic and molecular spectroscopy, photo-induced processes

Photofragmentation of dAMP- in a cryogenic ion trap

Christian Sprenger; Samuel White; Miriam Westermeier; Eric Sebastien Endres; Roland Wester

University of Innsbruck

As one of the building blocks of DNA, dAMP is vital for life as we know it. Previous studies have been performed that focused on the study of the breakup process of the molecule from CID [1] or from photofragmentation [2]. A spectrum of the relative fragmentation cross section of deprotonated dAMP was previously done [3] at room temperature. In our current work we have measured a spectrum of the deprotonated dAMP anion in a cryogenic 16 pole wire ion trap at a temperature below 4 K.

Our setup uses a custom-built nano-electro-spray ionization source. From the ion source the ions are guided towards and confined in a cryogenic 16-pole wire trap [4]. As proven in [5] through quadrupole He tagging of protonated Glycine cations, our trap reaches exceptionally low temperatures, below 4 K, during operation. The content of the trap is mass separated using a Wiley-McLaren type reflectron time of flight spectrometer.

The used light source for this experiment was an Ekspla NT240 used to record the spectrum between 240 nm and 270 nm. In comparison to previous results we were able to observe previously unresolved structure in the spectrum. Furthermore, we measured the growth rates of fragments of the deprotonated dAMP as a function of the wavelength. Our results will be presented.

References

[1] D. Strzelecka, S. Chmielinski, S. Bednarek, J. Jemielity, J. Kowalska, Sci. Rep., 515, 441-451 (2018)

[2] S. S. Kumar, M. Pérot-Taillandier, B. Lucas, S. Soorkia, M. Barat, J. A. Fayeton, J. Phys. Chem. A, 115, 10383-10390 (2011)

[3] J. C. Marum, A. Halevi, J. M. Weber; Phys. Chem. Chem. Phys., 11, 1740-1751 (2009)

[4] K. Geistlinger, M. Fischer, S. Spieler, L. Remmers, F. Duensing, F. Dahlmann, E. Endres, R. Wester, Rev. Sci. Instrum. 92, 023204 (2021)

[5] K. Geistlinger, F. Dahlmann, T. Michaelsen, M. Ončák, E. Endres, R. Wester, J. Mol. Spectrosc., 379, 111479 (2021)

#A14: Atomic and molecular spectroscopy, photo-induced processes

Experimental Oscillator Strengths For Forbidden Lines In Fe II

Uldis Bērziņš¹; Artūrs Ciniņš¹; Jānis Sniķeris^{1,2}; José Eduardo Navarro-Navarrete³; Paul Martini³; Henning Schmidt³; Henrik Hartman⁴

¹ University of Latvia, Faculty of Science and Technology, Institute of Atomic Physics and Spectroscopy, LV-1004, Riga, Latvia

² Gothenburg University, Department of Physics, SE-41296, Gothenburg, Sweden

³ Stockholm University, Alba Nova University Centre, SE-10691 Stockholm, Sweden

⁴ Malmö University, Faculty of Technology, SE-20506 Malmö, Sweden

Metastable levels are responsible for parity forbidden lines occurring in many low-density astrophysical plasmas, found in e.g. gaseous nebulae, planetary nebulae, protostars, stellar chromospheres. Line ratios from forbidden lines are a reliable tool for diagnostics of temperature and density of low-density astronomical objects.

We have applied the laser probe technique [1] to singly ionized iron (Fe II) in the ion storage ring facility at the DESIREE laboratory [2]. The lifetimes of four metastable states were measured with about 10 % accuracy. In combination with branching fractions obtained from astrophysical spectra the transition probabilities will be determined.

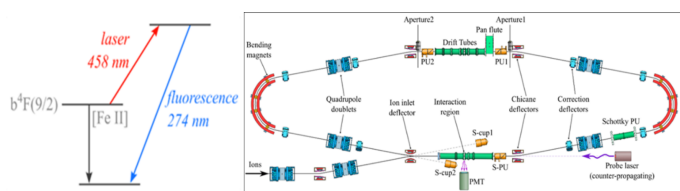


Fig.: A sketch showing the arrangement of the energy levels used for the probing technique and the wavelengths of the laser and fluorescence signals (left), and the ion storage ring and the detection scheme used at DESIREE (right).

We have demonstrated the successful measurement of the lifetime for the metastable states of a complex ion at DESIREE by the application of laser probing technique. We will report the measured lifetime data for four $3d^6 4s b^4 F$ levels.

Acknowledgements: U.B. and A.C. acknowledge the support by the Latvian Council of Science, Fundamental and Applied Research Project No. lzp-2023/1-0199: "The Laser Photodetachment Spectroscopy on Negative Ions".

[1] S Mannervik et al 2005 Phys. Scr. 49 (2005)

[2] Schmidt H. T., et al., Review of Scientific Instruments 84, 055115 (2013)

#A15: Atomic and molecular spectroscopy, photo-induced processes

Luminescence and scintillation properties of zinc-silicate glass ceramics

Vladimir Babin¹; Vítězslav Jarý¹; Petr Vařák²; Pavla Nekvindová²; Jan Mrázek³; Jakub Volf²

¹ Institute of Physics of the Czech Academy of Sciences, Cukrovarnická 10/112, 162 00 Prague, Czechia

² Department of Inorganic Chemistry, University of Chemistry and Technology, Technická 5, 166 28 Prague, Czechia

³ Institute of Photonics and Electronics of the Czech Academy of Sciences, Chaberská 57, 182 51 Prague, Czechia

Scintillating materials are finding their application as radiation detectors in many fields of human activity, such as medicine (TOF-PET), high-energy and space research, border crossing safety controls and others. The most used and studied materials so far are solid-state systems, such as CsI:Tl, Bi₄Ge₃O₁₂, Y(Lu)₃Al₅O₁₂:Ce, (Lu,Y)₂SiO₅:Ce and others. In recent years, distributed radiation sensors based on optical fibers have attracted attention, thanks to many advantages, such as resistance to electrical or magnetic interference, allowing the detection of a distant signal [1]. The creation of the inorganic composite nanoparticles and their distribution inside the glass matrix can improve the nanostructuring of the fiber core. Among others, glass-ceramics system with a general formula Na₂O-ZnO-Al₂O₃-SiO₂ is a perspective inorganic matrix. The dispersed crystalline nanoparticles possess significant scintillation properties. Due to the variability of the composition, it is possible to influence the formation of different phases as well as the size of the resulting nanoparticles [2].

The aim of the study is to investigate the structural, optical and scintillation properties of the mentioned glass-ceramics system. The efficient and fast emission located in the UV-visible spectral range under the ionizing radiation excitation was the goal of our research. The glass-ceramics compounds were prepared by the melt-quenching method, and the crystallization was induced by controlled heat treatment. The structure and optical properties of the prepared materials were characterized by the X-ray diffraction analysis and transmission electron microscopy. The steady-state and time-resolved photo- and radioluminescence properties were analyzed in broad energy and temperature range using a variety of excitation sources including also synchrotron radiation facility. The scintillating properties were evaluated, and the potential of prepared scintillating composites was assessed.

This work was supported by the Czech Science Foundation project no. GA23-05507S and DESY (Germany) projects for the research with synchrotron radiation no. I-20211395 EC, I-20231298 EC.

[1] J. Liu, X. Zhao, Y. Xu, H. Wu, X. Xu, P. Lu, X. Zhang, X. Zhao, M. Xia, J. Tang, G. Niu, "All-Inorganic Glass Scintillators: Scintillation Mechanism, Materials, and Applications", Laser Photonics Rev. 17, 2300006 (2023).

[2] V. Jarý, P. Vařák, V. Babin, J. Hrabovský, A. Michalcová, J. Volf, P. Nekvindová, J. Mrázek, "Scintillation properties of zinc-silicate glass-ceramics based on Zn₂SiO₄ willemite phase", Opt. Mater. 162, 116961 (2025).

#A16: Atomic and molecular spectroscopy, photo-induced processes

Coherent nonlinear four X-ray photon interaction with core-shell electrons

Ana Sofia Morillo Candas¹; Sven Augustin²; Eduard Prat²; Antoine Sarracini²; Jonas Knurr²; Serhane Zerdane²; Zhibin Sun²; Ningchen Yang³; Marc Rebholz⁴; Hankai Zhang³; Yunpei Deng²; Xinhua Xie²; Andrea Cannizzo⁵; Andre Al-haddad²; Kirsten Schnorr²; Christian Ott⁴; Thomas Feurer⁶; Christoph Bostedt³; Thomas Pfeifer⁴; Gregor Knopp²

¹ Max-Planck-Institut für Kernphysik (MPIK, Max Planck Institute for Nuclear Physics)

² Paul Scherrer Institute

³ Paul Scherrer Institute, École Polytechnique Fédérale de Lausanne

⁴ Max-Planck-Institut für Kernphysik

⁵ University of Bern

⁶ University of Bern, European XFEL

1. Introduction

The X-ray spectral range can address atomic scale (nm) spatial resolution at ultrafast time (fs) scales, with element specificity and site-selective excitation. Non-linear wave mixing techniques in this range, in particular four-wave mixing (FWM) methods, can thus provide information on the structural and electronic dynamics of atomic and molecular systems with unprecedented resolution. X-ray FWM brings the capability to study the electronic states coupling between spatially localized inner and/or core transitions among different sites of a quantum system or to study transport phenomena at the nanoscale. Whereas mixed XUV/X-ray - optical four-wave mixing and all-EUV have been successfully demonstrated in a transient grating (TG) configuration (see refs. [1-3] and refs. therein), non-linear all-X-ray four-wave mixing spectroscopy has been envisioned and theoretically described [4] but not yet realized experimentally, remaining as a long-awaited goal until now [5].

We demonstrate nonlinear X-ray four-wave mixing (XFWM) with all photons in the soft X-ray range (850-870 eV) using a non-collinear folded 'Box' or BoxCARS configuration [6]. In this robust configuration and obeying phase-matching, the X-ray photons generated by three interacting soft X-ray beams are emitted towards the fourth corner of a square, allowing for background-free detection. The signal could thus be clearly discriminated from the incoming beams and detected either by an in-line X-ray grating spectrometer ($\Delta E \approx 0.4$ eV), allowing for its spectral characterization or by recording the fluorescence from a YAG screen moved into the signal beam path, for its spatial characterization.

2. Results

SASE pulses from the Swiss Free Electron Laser (SwissFEL) are focused by a pair of KB mirrors into an in-vacuum gas-cell filled with a few hundreds mbar of Ne producing a coherent response from core-shell electrons. When scanning the FEL pink beam available at the Maloja end-station around the Ne K-absorption edge at ~ 870 eV, the YAG fluorescence shows a laser-like signal beam, well isolated from the incoming beams, which shows the maximum signal strength when approaching the pre-edge resonances of Ne. The signal generation efficiency, as defined by the ratio of signal photons that are scattered into the phase-matched direction and the incoming photons is in the order of 0.15 %, demonstrating an efficient signal generation.

The spectrally dispersed XFWM signals provide a rich map, comprising multiple contributions from neutral neon and its ions. The large set of parameters explored, including FEL intensity, gas pressure and pulse duration ranging from 30 fs down to 3 fs (rms), provides key information that allow us to disentangle the different origin of the XFWM signals, including resonantly-enhanced X-ray two-color processes. The measured results are compared to the available literature

on stimulated Raman X-ray scattering in Neon [7] and with the results of a dedicated model that accounts for the beam propagation and population changes during the X-ray pulse duration. We discuss in detail the measured and calculated 2D spectral maps, and how the correlation plots reflect the coupling between electronic states of neon, allowing us to distinguish these signals from X-ray lasing processes originated in the ions.

The general feasibility of non-collinear four-wave mixing in the X-ray range is demonstrated. The robustness of the setup, the strength of the signals and the spectral and spatial information achieved from the experiment implies a major breakthrough for the application of nonlinear X-ray wave mixing as a spectroscopic tool in general, and as basis for 2D X-ray correlation spectroscopy. In addition, preliminary time resolved signals and approaches to extend the proposed methodology to the time domain, based on two-colour mode available at the Athos branch of SwissFEL are introduced.

3. References

- [1] F. Bencivenga et al., "Four-wave mixing experiments with extreme ultraviolet transient gratings" *Nature* 520, 205 (2015).
- [2] F. Bencivenga, et al. "Nanoscale transient gratings excited and probed by extreme ultraviolet femtosecond pulses." *Sci. Adv.* 5(7) eaaw5805 (2019).
- [3] J.R. Rouxel, D. Fainozzi, R. Mankowsky, B. Rösner, G. Seniutinas, et al. "Hard x-ray transient grating spectroscopy on bismuth germinate" *Nat. Photon* 15(7), 499–503 (2021)
- [4] S. Tanaka and S. Mukamel "X-ray four-wave mixing in molecules" *J. Chem. Phys.* 116(5), 1877–1891 (2002)
- [5] A.S. Morillo-Candas, et al. "Coherent all X-ray four-wave mixing at core shell resonances." *arXiv preprint arXiv:2408.11881* (2024), <https://doi.org/10.48550/arXiv.2408.11881>
- [6] Y. Prior, "Three-dimensional phase matching in four-wave mixing" *Appl. Opt.* 19(11), 1741–1743 (1980)
- [7] C. Weninger, M. Purvis, D. Ryan, R.A. London, J.D. Bozek, C. Bostedt, A. Graf, G. Brown, J.J. Rocca, and N. Rohringer, "Stimulated Electronic X-Ray Raman Scattering" *PRL* 111, 233902 (2013).

#A17: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Erosion of the lunar surface by solar wind ions

Johannes Brötzner¹; Herbert Biber¹; Paul S. Szabo²; Martina Fellinger¹; Noah Jäggi³; Gyula Nagy¹; Eduardo Pitthan⁴; Daniel Primetzhofer⁴; Richard A. Wilhelm¹; André Galli⁵; Peter Wurz⁵; Friedrich Aumayr¹

¹ TU Wien, Institute of Applied Physics

² Space Sciences Laboratory, University of California

³ Material Science and Engineering Department, University of Virginia

⁴ Department of Physics and Astronomy, Uppsala University

⁵ Space Science and Planetology, Physics Institute, University of Bern

Solar wind sputtering is a key process driving material ejection from the lunar surface and contributing to the exosphere [1–5]. We present high-precision sputter yield measurements on Apollo 16 regolith samples, complemented by advanced 3D regolith modeling. Our results show that sputter yields for H and He ions at solar wind energies are nearly an order of magnitude lower than previously assumed. This significant reduction is attributed to surface roughness and porosity effects, which have not been adequately considered in past studies. Additionally, our data reveal discrepancies with numerical predictions that have otherwise been reliable for single minerals, suggesting that the properties of lunar regolith are not just a linear combination of its constituents.

By providing experimentally validated sputter yields for real lunar material, our work challenges existing exosphere models and offers a crucial benchmark for future studies. These findings have broad implications for interpreting data from upcoming missions like Artemis and

BepiColombo and for understanding space weathering on airless planetary bodies in general.

- [1] P. S. Szabo, et al., *Astrophys. J.* 891, 100, (2020)
- [2] P. S. Szabo, et al., *Geophys. Res. Lett.* 49, e2022GL101232, (2022)
- [3] H. Biber, et al., *Planetary Sci. J.* 3, 171, (2022)
- [4] N. Jäggi, et al., *Planetary Sci. J.* 4, 86, (2023)
- [5] N. Jäggi, et al., *Planetary Sci. J.* 5, 75, (2024)

#A18: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Ion-molecule reactions of acetylene inside helium nanodroplets: Formation of cationic benzene and other covalently bound hydrocarbons including PAHs

Florian Foitzik¹; Lisa Ganner¹; Vincent Richardson²;
Johannes Reichegger¹; Paul Scheier¹; Elisabeth Gruber¹

¹ Universität Innsbruck

² University of Liverpool

Ion-molecule reactions play a fundamental role in the chemical evolution of the Universe, driving the formation of increasingly complex organic molecules in various astrophysical environments. Reactions of ions with molecules are particularly dominant in the diffuse interstellar medium, in molecular clouds and in the photon-dominated regions, as the proportion of ionized molecules is particularly high in these parts of the Universe. On the other hand, the low temperatures in these environments also favor ion-molecule reactions - that are often characterized by very low or vanishing activation barriers - compared to neutral-neutral reactions.

One key molecular precursor of larger hydrocarbons and other organic molecules is acetylene (C_2H_2). Its widespread presence and the unique balance of stability and reactivity facilitate the bottom-up synthesis of larger carbon structures. Understanding the pathways leading from small hydrocarbons such as acetylene to bigger systems is crucial for unravelling the molecular complexity of the Universe [1].

Our group in Innsbruck investigates ion-molecule reactions inside helium nanodroplets. This matrix is ideal for studying chemical reactions of astrophysical relevance, as it is chemically inert and interacts weakly with the doped molecules. Furthermore, only barrier-free chemical reactions can take place in this environment due to its low equilibrium temperature of below 1K [2].

In this contribution, we present our findings on the formation of covalently bound molecular complexes by the sequential reaction of neutral acetylene molecules with $C_2H_2^+$. We report the formation of the ions $C_6H_6^+$, $C_8H_6^+$ and $C_{10}H_8^+$. While cationic benzene $C_6H_6^+$ has already been observed in experiments on electron impact ionization of neutral acetylene clusters [3], our method permits the detection of larger hydrocarbons formed by the onwards reaction of the benzene cation.

References

- [1] E. Pentsak et al., *ACS Earth Space Chem.* 8, 798-856 (2024)
- [2] S. Albertini et al., *Mass Spectrom. Rev.* 41, 529-567 (2022)
- [3] P. O. Momoh et al., *J. Am. Chem. Soc.* 128, 12408-12409 (2006)

#A19: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Impact of a smoothing parameter in breast radiotherapy planning

D. Szabó¹; Karoly Tokesi²; T. Ungvári¹

¹ 1Makrusovszky University Teaching Hospital, Szombathely, 9700, Hungary

² HUN-REN Institute for Nuclear Research

Radiotherapy remains a cornerstone of breast cancer treatment, with IMRT offering precise dose delivery while sparing healthy tissues. Treatment planning systems (TPS) frequently incorporate a smoothing function for intensity-modulated radiation therapy (IMRT) plans. This enables users to modify the intricacy of the beam fluence pattern in the x-y direction. Smoothing factor is a key parameter, affecting plan complexity, monitor units (MU) and treatment time.

This study evaluates the impact of SF on IMRT plan efficiency and quality. IMRT plans were generated for 21 patients with SF values ranging from 10 to 300, analyzing 126 plans using dose-volume histograms (DVH), modulation complexity score (MCS), and statistical testing (ANOVA with Bonferroni post hoc analysis). The planned dose was 15x2,67Gy. We calculated the modulating complexity score. It is imperative to minimize the complexity and enhance the robustness of the beam. This is due to the potential for a discrepancy between the planned and actual dose distribution. Our findings indicate that decreasing the smoothing parameters improves the plan quality but reduces the deliverability (MCS value), while increasing them decreases the complexity and plan quality. Results indicate that an SF range of 100-150 achieves optimal treatment efficiency while maintaining plan quality. This balance reduces treatment time and MU while ensuring adequate dose distribution and minimizing lung exposure. Optimizing SF can enhance personalized radiotherapy planning, improving clinical outcomes.

References

- [1] A.L. McNiven, M.B. Sharpe, T.G. Purdie, *Med. Phys.*, 37 505 (2010)
- [2] P. Niyas, K.K. Abdullah, M.P. Noufal, T. Sankaran Nair, 2016 *Radiol. Phys. Technol.*, 9 202 (2016)
- [3] V. Hernandez et al., 2020 *Radiother. Oncol.*, 153 26 (2020)

#A20: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Reactivity of Sea Salt Cluster Ions with Atmospherically Relevant Organic Acids in the Gas Phase

Jessica C. Hartmann¹; Sarah Keiler¹; Jia Yang Lim²; Yiqi Sheng²; Christian van der Linde¹; Marc Reimann¹; Sarah J. Madlener¹; Milan Ončák¹; Chi-Kit Siu²;
Martin Klemens Beyer¹

¹ Universität Innsbruck, Institut für Ionenphysik und Angewandte Physik

² City University Hong Kong, Department of Chemistry

Sea salt aerosols are among the most abundant natural aerosols and play a significant role for the climate. They mainly consist of sodium chloride, which is involved in chemical reactions in the atmosphere with atmospherically relevant trace gases. Such reactions are simulated in our experiments.

We use electrospray ionization (ESI) to produce gas-phase sodium chloride cluster ions. Atmospherically relevant acids, e.g. formic and pyruvic acid, are introduced as reaction gas into the ICR cell of a Fourier transform ion cyclotron resonance mass spectrometer (FT-ICR MS)

and reaction kinetics are recorded. We observe a sequential acid uptake by both anions and cations, accompanied by HCl release. We find a reactivity dependence on the proton affinity of the conjugate base. Interestingly, magic cluster sizes show a reduced reactivity for each acid used in our experiments. Detailed quantum chemical calculations reveal how a weak organic acid is able to displace HCl, known to be a strong acid.

#A21: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Apparatus for preparing conformationally pure gas-phase biomolecular clusters

Bendegúz Szihalmi¹; Thomas ten Napel¹; Marcelo Goulart²; Thomas Schlathölter¹

¹ University of Groningen, Zernike Institute for Advanced Materials, 9747 AG Groningen, Netherlands

² University of Groningen, University College Groningen, 9718 BG Groningen, Netherlands

Over the last years, our team has employed a combination of electrospray ionization with radiofrequency ion guiding and trapping, to prepare targets of mass-selected trapped gas-phase biomolecular ions for photoexcitation/photoionization experiments using synchrotron, free electron laser or conventional laser beams [1] but also for collision experiment using MeV ions [2]. A recurrent problem in studies involving large molecular systems is the fact that they usually occupy a large conformational space, even under cryogenic conditions.

Conformationally separation of gas phase biomolecules has historically been achieved using drift tubes, where bunches of molecular ions drift through an inert gas under the influence of an electric field. The ion drift velocity can then be directly related to its geometric cross section. Typically however, these tubes need to be several meters long and require kV potentials which makes this approach problematic for interfacing with synchrotron or heavy ion beamlines where floorspace is limited and flexibility is required.

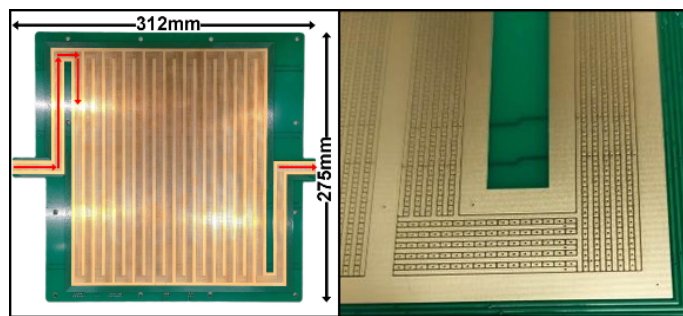


Fig.: Photographs of the bottom printed circuit board of the travelling wave IMS system featuring DC guard electrodes, RF guiding electrodes and traveling wave pixels. Red arrows represent the direction of ion transport.

To overcome these issues our team has implemented an alternative ion-mobility approach based on radiofrequency ion guiding. Using the method pioneered by the Smith group at PNNL [3] the ions are guided by means of electrodes on a printed circuit board (see figure). This approach does not require high voltage gradients since the ions are transported using traveling waves. By using a serpentine path an overall pathlength of several meters can be collapsed into a compact instrument (see figure). This apparatus allows our team to produce m/q selected and conformationally pure beams of protonated and deprotonated biomolecular ions that can be easily interfaced with laser, synchrotron and MeV ion beamlines.

In the near future, we plan to use MeV carbon ions from the IRRSUD

facility at GANIL/France to investigate collisions with conformer selected DNA.

References:

- [1]: W. Li, O. Kavatsyuk, W. Douma, X. Wang, R. Hoekstra, D. Mayer, M. Robinson, M. Gühr, M. Lalande, M. Abdelmouleh, M. Ryszk, J.-C. Pouilly, T. Schlathölter, 2021 Chemical Science 12 13177
- [2]: M. Lalande, M. Abdelmouleh, M. Ryszk, V. Vizcaino, J. Rangama, A. Méry, F. Durantel, T. Schlathölter, and J.-C. Pouilly, 2018 Physical Review A 98 062701
- [3]: L. Deng, Y. M. Ibrahim, E. S. Baker, N. A. Aly, A. M. Hamid, X. Zhang, X. Zheng, S. V. B. Garimella, I. K. Webb, S. A. Prost, J. A. Sandoval, R. V. Norheim, G. A. Anderson, A. V. Tolmachev, R. D. Smith, 2016 ChemistrySelect, 1, 2396.

#A22: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Anyonization of bosons

Sudipta Dhar¹; Botao Wang²; Milena Horvath¹; Amit Vashisht²; Yi Zeng¹; Mikhail Zvonarev³; Nathan Goldman²; Yanliang Guo¹; Manuele Landini¹; Hanns-Christoph Nägerl¹

¹ University of Innsbruck

² Université Libre de Bruxelles

³ Université Paris-Saclay

Anyons [1,2] are low-dimensional quasiparticles that obey fractional statistics, hence interpolating between bosons and fermions. In two dimensions, they exist as elementary excitations of fractional quantum Hall states and they are believed to enable topological quantum computing. One-dimensional (1D) anyons have been theoretically proposed, but their experimental realization has proven to be difficult. In this talk, we report the observation [3] of emergent anyonic correlations in a 1D strongly-interacting quantum gas, resulting from the phenomenon of spin-charge separation. A mobile impurity provides the necessary spin degree of freedom to engineer anyonic correlations in the charge sector and simultaneously acts as a probe to reveal these correlations. Starting with bosons, we tune the statistical phase to transmute bosons via anyons to fermions and observe an asymmetric momentum distribution, hallmark of anyonic correlations. Going beyond equilibrium conditions, we observe dynamical fermionization of the anyons [4], where the momentum distribution of an expanding sample of 1D hardcore anyons following a trap quench becomes indistinguishable from that of a non-interacting, spin-polarized Fermi gas over time, irrespective of the statistical phase. Our work opens up the door to the exploration of non-equilibrium anyonic phenomena in a highly controllable setting.

[1] J. M. Leinaas and J. Myrheim, On the theory of identical particles, *Il Nuovo Cimento B* (1971-1996) 37, 1 (1977).

[2] F. Wilczek, Quantum mechanics of fractional-spin particles, *Phys. Rev. Lett.* 49, 957 (1982).

[3] S. Dhar, B. Wang, M. Horvath, A. Vashisht, Y. Zeng, M.B. Zvonarev, N. Goldman, Y. Guo, M. Landini and H.C. Nägerl, 2024. Anyonization of bosons. *arXiv preprint arXiv:2412.21131*.

[4] A. del Campo, Fermionization and bosonization of expanding one-dimensional anyonic fluids, *Phys. Rev. A* 78, 045602 (2008).

#A23: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Bloch Oscillations of a Soliton in a 1D Quantum Fluid

Guillaume Brochier; Franco Rabec; Guillaume Chauveau; Sylvain Nascimbene; Jean Dalibard; Jérôme Beugnon

Laboratoire Kastler Brossel

Bloch oscillations are a striking feature of the counterintuitive motion of particles created by a lattice potential [1]. However, this phenomenon does not require the presence of a lattice, nor is it limited to single-particle physics. One can reproduce such an effect with a system, possibly many-body, that is translationally invariant, provided that the dispersion relation remains periodic [2].

A notable example of this phenomenon is magnetic solitons, which can be mapped onto an immiscible spin mixture in a quasi-1D Bose gas. We report on the observation of such Bloch-like oscillations, which prove to be analogous to Josephson physics [3]. Our experimental investigation encompasses both strict and periodic boundary conditions, the latter of which highlights the importance of the phase coherence of the quantum bath and the associated topology.

[1] F. Bloch, Z. Phys. 52, 555 (1929).

[2] D.M. Gangardt and A. Kamenev, Phys. Rev. Lett. 102, 070402 (2009).

[3] S. Bresolin, A. Roy, G. Ferrari, A. Recati, and N. Pavloff, Phys. Rev. Lett. 130, 220403 (2023).

#A24: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Optical excitation and stabilization of ultracold field-linked tetratomic molecules

Bijit Mukherjee; Michał Tomza

Faculty of Physics, University of Warsaw

In recent years, shielding of ultracold molecules [1, 2] from close collisions inside an optical dipole trap has brought remarkable achievements in cooling molecules to quantum degeneracy [3, 4]. Shielding can be achieved by an external static electric field or a near-resonant microwave. This external field also allows the creation of weakly bound tetratomic molecules ("tetramers") from a pair of ultracold diatomic molecules. Such tetramers have been realized recently for shielded NaK molecules using an external microwave field [5]. These tetramers are termed field-linked (FL) molecules as an external field is necessary to create them.

The FL tetramers that have been realized are very shallow with binding energies of the order of 100 kHz. The motivation of this work is to develop a methodology to create deeper bound tetramers starting from the loosely bound FL tetramers. Our methodology draws the ideas of photoassociation of ultracold atoms to diatoms followed by stabilization to ground state, and stimulated Raman adiabatic passage (STIRAP) transfer of weakly bound diatoms to deeply bound ground vibronic molecules. We envisage similar routes of creating deeply bound tetramers starting from the weakly bound states or a pair of colliding diatoms. We consider static-electric-field shielded alkali diatomic molecules initially in their ground vibronic $|X^1\Sigma^+, v=0\rangle + |X^1\Sigma^+, v=0\rangle$ (hereafter X+X) pair state. We identify the excited vibronic manifold $|X^1\Sigma^+, v=0\rangle + |b^3\Pi_0, v'=0\rangle$ (hereafter X+b) for photoassociation and an intermediate state for STIRAP transfer to deeply bound states in the X+X manifold. For this, we develop shielding methods for X+b and predict Frank-Condon factors (FCFs)

between FL states of X+b and X+X. We also predict photoassociation spectra for shielded molecules to form FL tetramers in X+b manifold. We obtain highly tunable FCFs between ground and excited tetramer states and promising photoassociation spectra. Our theoretical results should guide future experiments for stabilizing weakly bound ultracold tetramers.

References

1. G. Wang and G. Quémener, New J. Phys. 17, 035015 (2015).
2. T. Karman and J. M. Hutson, Phys. Rev. Lett. 121, 163401 (2018).
3. A. Schindewolf et al., Nature 607, 677 (2022).
4. N. Bigagli et al., Nature 631, 289 (2024).
5. X.-Y. Chen et al., Nature, 626, 283 (2024).

#A25: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Ultracold Coherent Control of molecular collisions at a Förster resonance

Thibault Delarue¹; Goulven Quémener²

¹ Laboratoire Aimé Cotton (LAC), université Paris-Saclay

² Laboratoire Aimé Cotton, CNRS, Université Paris-Saclay

Ultracold coherent control of molecular collisions at a Förster resonance

The advent of ground-state controlled ultracold dipolar molecules in dense gases has opened many exciting perspectives for the field of ultracold matter. When the molecules are dipolar, their extremely controllable properties have inspired many theoretical proposals for promising quantum applications, such as quantum simulation/information processes, quantum-controlled chemistry and test of fundamental laws.

Ultracold molecules can be used to probe chemical reactions with an unprecedented control at the quantum level. This was done recently with the chemical reaction $KRb + KRb \rightarrow K_2 + Rb_2$ at ultracold temperatures. All the fragments of an ultracold chemical reaction, from reactants to products, including intermediate complexes, can now be observed [1]. The state-to-state rotational distribution of the products can be measured [2] and the rotational parities of the molecular products can be controlled with a magnetic field [3, 4].

We explore here the ideas of coherent control [5] applied to current experiments of ultracold chemical reactions. By using a microwave to prepare ultracold dipolar molecules in a quantum superposition of three stationary states (qutrit) and by using a static electric field to make collisional states degenerate, we predict that one can observe interferences in the rate coefficients of ultracold molecules. This work provides a realistic and concrete experimental set-up for current experiments to observe interferences and coherent control in ultracold collisions [6].

References

- [1] M.-G. Hu et al., *Direct observation of bimolecular reactions of ultracold KRb molecules*, Science 366, 1111 (2019).
- [2] Y.Liu et al., *Precision test of statistical dynamics with state-to state ultracold chemistry*, Nature 593, 379 (2021).
- [3] M.-G. Hu et al., *Nuclear spin conservation enables state-to-state control of ultracold molecular reactions*, Nat. Chem. 13, 435 (2021).
- [4] G. Quémener et al., *Model for nuclear spin product-state distributions of ultracold chemical reactions in magnetic fields*, Phys. Rev. A 104, 052817 (2021).

[5] M. Shapiro and P. Brumer, *Coherent control of molecular dynamics*, Rep. Prog. Phys. 66, 859 (2003).

[6] T. Delarue and G. Quémener, *Ultracold coherent control of molecular collisions at a Förster resonance*, Phys. Rev. A 109, L061303 (2024).

#A26: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Combining atomic ensembles with single atoms to realize collectively enhanced detection using EIT

Lew Schöne¹; Amar Bellahsene¹; Swayangdipta Bera¹; Clément Gradziel¹; Maximilian Müllenbach¹; Shuzhe Yang¹; Tom Bienaimé²; Shannon Whitlock¹

¹ Université de Strasbourg

² CNRS Researcher

Arrays of single atoms in optical tweezers are a strong contestant in the race for quantum computing and simulation platforms [1]. Besides their strengths - scalability, environmental isolation and adaptability - the system still lags speed when it comes to qubit manipulation and readout. This project aims to implement a new fast detection scheme to enable measurements on the microsecond timescale. In the group of Prof. Whitlock in Strasbourg we have experience with arrays of atomic ensembles in microtraps [2]. We now want to combine ensembles with single atoms to realize collectively enhanced detection using Rydberg electromagnetically induced transparency [3] to detect the state of a single atomic qubit. The big challenges of this measurement scheme are the preparation of the atomic ensemble and the single atom in neighboring tweezers, as well as an optimized interaction and readout sequence. Implemented on a potassium quantum gas machine, this new detection method will enable fast and state sensitive measurements.

References

1. M. Morgado and S. Whitlock, AVS Quantum Science 3, no. 2 (May 3, 2021): 023501
2. Yibo Wang et al., Npj Quantum Information 6, no. 1 (June 17, 2020): 1–5
3. Wenchao Xu et al., Physical Review Letters 127, no. 5 (July 27, 2021): 050501

#A27: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Dipolar Supersolids as a Platform for Tunable Josephson Junctions

Natalia Masalaeva; Russell Bisset

Institut für Experimentalphysik, Universität Innsbruck, Innsbruck, Austria

We investigate binary dipolar supersolids as a platform for tunable Josephson junctions in atomtronics. By rotating a binary dipolar condensate, we induce the nucleation of quantized vortices, which act as self-assembled weak links between localized superfluid domains. In our work, we show that these weak links resemble Dayem bridges in superconductors and aperture arrays in liquid helium.

We introduce the concept of core currents, where one superfluid component penetrates the vortex cores of the other under an applied phase gradient, analogous to voltage-driven transport in superconducting circuits. By analyzing the current-phase relations, we identify distinct tunneling and hydrodynamic regimes, which can be controlled by tuning parameters such as atom number and scattering length.

Our findings establish binary supersolids as a promising platform for atomtronic Josephson junctions, bridging supersolidity and quantum transport in ultracold gases.

#A28: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

All Optical Formation of Bose-Einstein Condensate near Dielectric Surface

Hayato Kawamura; Ryota Hashimoto; Taro Mashimo; Satoshi Tojo

Department of Physics, Chuo University

Precise manipulation of a quantum degenerate gas can work for a quantum sensing for investigation of atom surface interactions owing to their high-sensitivity to electromagnetic fields such as van der Waals and Casimir-Polder potentials [1, 2]. In the vicinity of dielectric surface, particularly in the evanescent field region, theoretical models suggest that transition probabilities of optically forbidden transitions are enhanced more than several orders of magnitude [3].

We have experimentally investigated atom-surface interactions using

⁸⁷Rb $F = 1$ Bose-Einstein condensate (BEC). Pre-cooled atoms are loaded into an optical dipole trap [4] and transported to a glass surface region. We vertically adjust the position of the focal point of the trapping light in standing waves formed by the incident and reflected trapping beams at the distance of $10\ \mu\text{m}$ from the surface. After the transportation, we decrease the temperature of the atoms by the evaporative cooling in the standing wave potential crossed with a vertically trap beam and create a BEC in the trap.

We study the dynamics of a BEC near a dielectric surface depending on evolution time and report on the oscillation behaviors of the BEC in the vicinity of the surface.

References

- [1] Athanasios Laliotis, Bing-Sui Lu, Martial Ducloy, Daniel Bloch, and David Wilkowski, AVS Quantum Sci. 3, 043501 (2021).
- [2] J. M. Obrecht, R. J. Wild, M. Antezza, L. P. Pitaevskii, S. Stringari, and E. A. Cornell, Phys. Rev. Lett. 98, 063201 (2007).
- [3] Kosuke Shibata, Satoshi Tojo, and Daniel Bloch, Optics Express 25, 9476 (2017).
- [4] Taro Mashimo, Masashi Abe, and Satoshi Tojo, Phys. Rev. A 100, 063426 (2019).

#A29: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Interactions between metastable triplet-state helium dimers

Dibyendu Sardar¹; Michał Tomza²

¹ University of Warsaw

² Faculty of Physics, University of Warsaw

Over the last two decades, a drift of interest in molecular science has steered towards the creation and manipulation of ultracold molecules. The intricate internal structure of molecules due to the presence of rotational and vibrational degrees of freedom attracts more attention because of their application in quantum simulation, precision measurement, and ultracold chemistry. To date, a limited number of studies on the collisional properties of ultracold molecules are available, where ultracold noble gas molecules are still largely unexplored.

This project explores ultracold molecular interactions and collisional dynamics involving metastable noble gas helium molecules in a spin-polarized triplet state, $^3\Sigma_u^+$. We use state-of-the-art ab initio quantum chemistry methods to understand the interactions between two metastable He₂ molecules by calculating the potential energy surfaces (PESs) both in their ground and excited electronic states. Our analysis identifies a global minimum with D_{2d} symmetry having a depth of 3100 cm⁻¹, supporting multiple ro-vibrational bound states. The PES for this global minimum undergoes curve crossings with other symmetry states arising from the excited electronic state.

Once we finish a complete multidimensional PES for the helium tetramer, our next aim is to calculate the full-dimensional quantum scattering calculations for He₂ ($^3\Sigma_u^+$) + He₂ ($^3\Sigma_u^+$) collisions to measure the scattering length and to investigate state-selective energy-transfer processes. The metastable He₂ is a light system with four electrons, its PES and scattering properties can be computed with high accuracy. On top of the immediate importance of He₂ ($^3\Sigma_u^+$), this molecule is an ideal system for laser cooling and a perfect candidate for precision measurements. Interactions and cold collisions between He₂ molecules are also useful for evaporative cooling, analyzing the formation of the Bose-Einstein condensate of metastable helium molecules.

[1] S. L. Cornish, M. R. Tarbutt, and K. R. A. Hazzard, *Nat. Phys.*, **20**, 730, (2024).

[2] T. E. Wall, *J. Phys. B: At. Mol. Opt. Phys.*, **49**, 243001, (2016).

[3] T. Karman, M. Tomza, and J. Pérez-Ríos, *Nat. Phys.*, **20** 722, (2024).

#A30: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

High fidelity control of a many-body Tonks-Girardeau gas with an effective mean-field approach

Muhammad Hasan¹; Thomas Fogarty²; Jing Li³; Andreas Ruschhaupt³; Thomas Busch²

¹ Institute of Atomic and Molecular Sciences, Academia Sinica

² OIST, Japan

³ UCC, Ireland

Shortcuts to adiabaticity (STA) are powerful tools that can be used to control quantum systems with high fidelity. They work particularly well for single particle and noninteracting systems which can be described exactly and which possess invariant or self-similar dynamics.

However, finding an exact STA for strongly correlated many-body systems can be difficult, as their complex dynamics may not be easily described, especially for larger systems that do not possess self-similar solutions. Here, we design STAs for one-dimensional bosonic gas in the Tonks-Girardeau limit by using a mean-field approach that succinctly captures the strong interaction effects through a quintic nonlinear term in the Schrödinger equation. We show that for the case of the harmonic oscillator with a time-dependent trap frequency, the mean-field approach works exactly and recovers the well-known STA from literature. To highlight the robustness of our approach, we also show that it works effectively for anharmonic potentials, achieving higher fidelities than other typical control techniques.

[1]. Muhammad S. Hasan, T. Fogarty, J. Li, A. Ruschhaupt, and Th. Busch, *Phys. Rev. Research* **6**, 023114 (2024)

#A31: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Barium Fluoride Deceleration Using Temporary Ionization

Martin Collignon; Hans Lignier; Bruno Viaris de Lesegno; Matteo Marciano

Laboratoire Aimé Cotton, Université Paris-Saclay / CNRS

Due to their complex structure, molecules are interesting systems for applications in various fields such as quantum chemistry or precision measurements. But it also implies more difficult cooling techniques than for atoms.

This experiment on Barium Fluoride (BaF) aims at decelerating a supersonic molecular beam by using the electric force on ions, which is much more intense than the dipolar force commonly used on molecules in other slowing techniques. It thus requires fewer space and weaker electric fields compared to other techniques. For instance, applying a field of a few volts/cm is enough to decrease from 600m/s to almost zero velocity the ions in about 10 microseconds and over a few millimeters.

This deceleration process is composed of three main steps: the ionization of the molecules in BaF⁺ or BaF⁻, the ions deceleration by an electric field pulse and the neutralization. Whatever the type of formed ion, it is necessary to ensure an electron capture: for the neutralization of BaF⁺ or for the formation of BaF⁻ from BaF. In both cases, this process will happen through the interaction of the molecules (BaF and BaF⁺) with a Rydberg atom beam, for which electrons are weakly bound.

These processes will be studied experimentally by probing the internal and external states of the neutral and ionic forms of BaF as a function of the different control parameters available such as the density of Rydberg atoms, the choice of their quantum number and the initial molecular state).

#A32: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Towards the Simulation of Complex Models of Quantum Magnetism with Electromagnetic Dipoles

Niclas Höllrigl¹; Marian Kreyer²; Emil Kirilov³; Rudolf Grimm²

¹ University of Innsbruck

² Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria

³ Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria. Institut für Experimentalphysik, Universität Innsbruck, Austria

We present our current progress towards a quantum gas microscope apparatus for experiments with ultracold dysprosium atoms exhibiting long-range dipole-dipole interactions (DDI). In addition to its large permanent magnetic dipole moment, Dy offers a set of closely-spaced opposite parity states (OPS), that can be dressed by microwave radiation to give rise to a tunable electric DDI. This approach can be used to simulate complex spin models (such as the XYZ model) and avoids some of the technical challenges of other platforms (e.g. heteronuclear molecules). The primary tool of our apparatus is a high-resolution microscope [1]. We show our current progress towards loading and positioning the atomic sample in a single 2D plane coincident with the focal plane of the microscope with the help of a beat-note lattice [2]. For achieving single-site imaging resolution we recently added an incoherent light source, which will be used to engineer a 2D matter-wave magnifier [3]. Recently, this source has also been used together with a digital micromirror device (DMD) to shape arbitrary trapping potentials. Furthermore, we show preliminary spectroscopic data towards the efficient population of the OPS via stimulated Raman adiabatic passage (STIRAP).

[1] G. Anich et al., Phys. Rev. A 110, 023311 (2024)

[2] L. Masi et al., Phys. Rev. Lett. 127, 020601 (2021)

[3] L. Asteria et al., Nature 12, 599 (2021)

#A33: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Two-Photon Optical Shielding of Collisions Between Ultracold Polar Molecules

Gohar Hovhannesian¹; Charbel Karam²; Romain Vexiau¹; Maxence Lepers²; Nadia Bouloufa-Maafa¹; Olivier Dulieu¹

¹ Laboratoire Aimé-Cotton, CNRS

² Laboratoire Interdisciplinaire Carnot de Bourgogne, CNRS, Université de Bourgogne Franche-Comté, 21078, Dijon, France

The full understanding and modeling of few-body systems remains a long-standing challenge in several areas of science, particularly in quantum physics. The ability to create and manipulate dilute gases at ultracold temperatures, composed of particles with kinetic energies $E = k_B T \ll 1$ mK opened novel opportunities in this respect. The growing availability of quantum gases of ultracold polar molecules (i.e., possessing a permanent electric dipole moment in their own frame) in various laboratories revealed a very peculiar situation in the context of few-body physics: At ultracold energies, two such molecules in their absolute ground level (i.e., in the lowest rovibrational and hyperfine level of their electronic ground state) collide with a universal collisional rate,

even if they have no inelastic or reactive energetically allowed channels, so they leave the molecular trap with a short characteristic time. Such a four-body system, which might appear relatively simple at first glance, is not yet fully characterized. Rather than attempting to fully describe this four-body system in order to identify the exact cause of the universal loss rate, one can design protocols where molecules do not reach short distances during their collision.

The goal of our theoretical work is to find ways to suppress inelastic or reactive processes between colliding particles in ultracold quantum gases [1]. Besides microwave coupling recently used for collisional shielding [2,3,4], we propose a method to engineer repulsive long-range interactions between ultracold ground-state molecules using optical fields, thus preventing short-range collisional losses. The process is modeled for a two-photon Raman resonance blue-detuned with respect to excited electronic state. It allows taking advantage of optically driven transitions including insensitivity to polarization and flexibility in the choice of electronic states, while suppressing undesired off-resonant photon scattering which was present in the previously proposed one-photon optical shielding (1-OS) [5]. The proposed protocol, exemplified for $^{23}\text{Na}^{39}\text{K}$, should be applicable to a broad class of polar diatomic molecules as well [6].

[1] Guo, M., Zhu, B., Lu, B., Ye, X., Wang, F., Vexiau, R., ... & Wang, D. (2016). Creation of an ultracold gas of ground-state dipolar Na 23 rb 87 molecules. Physical review letters, 116(20), 205303.

[2] Lassablière, L., & Quémener, G. (2018). Controlling the scattering length of ultracold dipolar molecules. Physical Review Letters, 121(16), 163402.

[3] Karman, T., & Hutson, J. M. (2018). Microwave shielding of ultracold polar molecules. Physical review letters, 121(16), 163401.

[4] Schindewolf, A., Bause, R., Chen, X. Y., Duda, M., Karman, T., Bloch, I., & Luo, X. Y. (2022). Evaporation of microwave-shielded polar molecules to quantum degeneracy. Nature, 607(7920), 677-681.

[5] Xie, T., Lepers, M., Vexiau, R., Orbán, A., Dulieu, O., & Bouloufa-Maafa, N. (2020). Optical shielding of destructive chemical reactions between ultracold ground-state NaRb molecules. Physical Review Letters, 125(15), 153202.

[6] Karam, C., Vexiau, R., Bouloufa-Maafa, N., Dulieu, O., Lepers, M., zum Alten Borgloh, M. M., ... & Karpa, L. (2023). Two-photon optical shielding of collisions between ultracold polar molecules. Physical Review Research, 5(3), 033074.

#A34: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

High-fidelity quantum logic state detection of single trapped molecular ions

Mikolaj Roguski¹; Aleksandr Shlykov¹; Richard Karl¹; Meissa Diouf¹; Ziv Meir²; Umesh Joshi¹; Stefan Willitsch¹

¹ University of Basel

² Weizmann Institute of Science

Quantum-logic protocols have emerged as an important tool for characterization of trapped atomic and molecular ions with complex energy-level structures. In such schemes, the internal state of the target ion is mapped onto a state of a co-trapped logic ion with accessible transitions, typically via shared motional modes.

Here, we report on quantum-logic state detection of N_2^+ with 99.99% fidelity for as few as nine experimental repetitions - an order-of-magnitude improvement over our previous results [1]. By combining experiments and simulations, we identify the fidelity-limiting role of the population in the motional modes not directly involved in the state readout and associate it with Debye-Waller effects. The enhanced detection fidelity reduces the experimental duty cycle and improves sensitivity towards higher molecular states that could be potentially identified under similar experimental conditions.

Our current efforts focus on precision spectroscopy and coherent manipulation of single molecules, which can be used to test fundamental and beyond-standard-model theories, develop THz-range molecular clocks, and investigate state-resolved single-molecule collisions.

[1] I. M. Sinal, Z. Meir, K. Najafian, G. Hegi, S. Willitsch, *Science*, 367, 1213–1218 (2020).

#A35: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Structure, stability and superfluidity of Bose-Bose bulk mixtures and droplets in quasi-2D confinement and optical lattices

Leandra Vranjes Markic¹; Ivan Poparic¹; Nikola Vukman¹; Kresimir Dzelalija¹; Petar Stipanovic¹; Robert Zillich²; Ferran Mazzanti³; Jordi Boronat³

¹ University of Split, Faculty of Science

² Johannes Kepler University Linz

³ Universidad Politecnica de Catalunya

We present the study of dilute Bose-Bose mixture of two hyperfine states of ³⁹K confined by an external harmonic potential in one spatial direction extending the recent research of some of the authors [1] towards the two-dimensional limit, in which the liquid phase is formed whenever the intraspecies interactions are repulsive and the interspecies one is attractive [2].

First, we study the bulk mixture using quantum Monte Carlo methods at T=0 and obtain equations of state for several confinement strengths. Attractive interspecies and repulsive intraspecies interactions are modeled with potentials that include information on s-wave scattering length and effective range. Based on the quantum Monte Carlo equation of state we develop a two-dimensional density functional for each confinement strength and use it together with the local density approximation to determine density profiles of self-bound drops and the formation of vortices. For weaker confinement, droplet profiles obtained using two-dimensional density functional agree well with the profiles previously obtained using three-dimensional functionals [1]. As the confinement strength is increased the number of particles needed to form a droplet with saturated density is significantly decreased. This is accompanied with the decrease of the critical number of atoms needed to form a stable vortex. In selected cases, we compare our results with Lee–Huang–Yang beyond mean-field theory predictions.

Adding the optical lattice in two directions perpendicular to the harmonic confinement, we study the changes in droplet stability and density profiles as the strength of the optical lattice is increased. Additionally, we report the quantum Monte Carlo results of bulk mixture in optical lattices, including the equations of state and the evolution of superfluidity with the increase of lattice depth.

[1] A. Sanuy, et al., *PRA* 109, 013313 (2024).

[2] D. S. Petrov and G. E. Astrakharchik, *Phys. Rev. Lett* 117, 100401 (2016).

#A36: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Modeling weakly bound few-body systems of ultracold quantum mixtures

Petar Stipanovic¹; Leandra Vranjes Markic¹; Jordi Boronat²

¹ University of Split, Faculty of Science

² Departament de Física, Universitat Politècnica de Catalunya

We present a theoretical study of weakly bound quantum systems in ultracold Bose-Fermi mixtures, focusing on their halo character and universal scaling behavior [1,2]. Using Variational Monte Carlo (VMC) and Diffusion Monte Carlo (DMC) methods, we compute ground-state binding energies and spatial distributions of few-body states formed near a Feshbach resonance in the ²³Na–²³Na–⁴⁰K system [1]. We develop and analyze interaction models to observe how repulsive intraspecies interactions make a system dilute. We explore universal properties to compare our findings with established universality curves from molecular halo clusters and discuss the implications for heteronuclear mixtures.

[1] P. Stipanović, L. Vranješ Markić, I. Bešlić & J. Boronat: Universality in molecular halo clusters, *Physical review letters*, 113, 25 (2014).

[2] P. Stipanović, L. Vranješ Markić & J. Boronat: Van der Waals five-body size-energy universality, *Scientific reports*, 12, 10368 (2022).

[3] Alexander Y. Chuang, Huan Q. Bui, Arthur Christianen, Yiming Zhang, Yiqi Ni, Denise Ahmed-Braun, Carsten Robens & Martin W. Zwierlein: Observation of a Halo Trimer in an Ultracold Bose-Fermi Mixture, arXiv:2411.04820v1 (2024).

#A37: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Collective effects in thermometry and cooling of trapped ions

Ivan Vybornyi; Klemens Hammerer

Leibniz University Hannover

Crystals of cold trapped ions are a promising platform for quantum technology and for studying the quantum many-body problem as a well-controlled toy many-body system. In modern state-of-the-art experiments, managing the entropy of large Coulomb crystals becomes challenging due to the exponential scaling of the Hilbert space with the number of trapped ions. In particular, as we demonstrate, collective effects must be taken into account and play an important role in both motional temperature measurement and the cooling process. Regarding the latter, the possible influence of collective effects has been debated in the literature in recent years. In my talk, I will present a thermometry protocol for large ion crystals that accounts for the emerging collective dynamics [1] and describe a mechanism that enhances the cooling of collective modes as more ions are added to the crystal.

[1] I.Vybornyi et. al, *PRX Quantum* 4, 040346 (2023)

#A38: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Vortices in a dipolar supersolid and single erbium atoms in optical tweezers

Manfred Mark; Eva Casotti; Elena Poli; Clemens Ulm; Lauritz Nathanael Klaus; Andrea Litvinov; Daniel Schneider Grün; Riccardo Donofrio; Arina Tashchilina; Francesca Ferlino

Institut für Experimentalphysik

Supersolids are exotic states of matter that spontaneously break two symmetries: gauge invariance through the phase-locking of the wavefunction, and translational symmetry owing to the emergence of a crystalline structure. In a first part, we report on the theoretical study and experimental observation of vortices in a dipolar supersolid of Dysprosium [1]. When rotated, the supersolid phase shows a mixture of rigid-body and irrotational behavior, highlighting a fundamental difference between modulated and unmodulated superfluids.

Neutral atoms in optical tweezers are one of the most promising platforms for quantum simulation and computation as they offer the implementation of arbitrary geometries, dynamical reconfiguration, generation of free-defects arrays and controllable long-range coupling via Rydberg-mediated interactions. In the second part, we will present our latest results on the successful loading and detection of single erbium atoms in a linear array of optical tweezers [2]. By implementing two complementary techniques for single atoms detection - narrow-linewidth non-destructive and broad-linewidth ultrafast imaging - we characterized the differential light shift for the intercombination line of erbium, and we investigated light-assisted collisions (LAC) and heating-induced losses.

[1] Observation of vortices in a dipolar supersolid, E. Casotti, E. Poli, L. Klaus, A. Litvinov, C. Ulm, C. Politi, M. J. Mark, T. Bland, F. Ferlino, *Nature*, 635, 327–331, 2024

[2] Optical Tweezer Arrays of Erbium Atoms, D. S. Grün, S. J. M. White, A. Ortu, A. Di Carli, H. Edri, M. Lepers, M. J. Mark, F. Ferlino, *Phys. Rev. Lett.*, 133, 223402, 2024

#A39: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Role of electron-impact charge transfer excitations of molecular and quasimolecular ions in the relaxation processes in noble gas mixture plasmas

Alexander Narits; Konstantin Kislov; Vladimir Lebedev

P.N. Lebedev Physical Institute of the Russian Academy of Sciences

The plasmas of noble gas mixture, routinely used as the active media of the powerful gas lasers, as well as of the sources of UV- and VUV-range radiation, contains, apart from the electrons, atomic ions and neutral atoms, also a fraction of homonuclear and heteronuclear molecular ions. Such heteronuclear ions have moderate to small dissociation energies in the range from 13.1 to 647 meV (for HeXe⁺ and HeNe⁺, respectively). As the IR and UV radiation sources above typically operate at room and elevated gas temperatures and the binding energies of the ions are small, the collisional and radiative processes involving the ions proceed often with the participation of the entire rovibrational spectrum, as well as the continuum of the internuclear motion. The heteronuclear BA⁺ ions feature the excited electronic charge transfer states which are described by AB⁺ configuration and

correlate in the dissociation limit with A + B⁺ collision system. It is well-known [1] that the transitions between the states with charge transfer character and the low-lying electronic terms of the heteronuclear rare gas ions result in the intense bands of the radiation in the UV, visible or VUV ranges, depending on the specific ion considered. In plasmas, similar transitions can be induced by the resonant collisions of the ions with the free electrons, BA⁺ + e → AB → AB⁺ + e, where the initial and the final states of the internuclear motion of the ions may be either bound or free. Such reactions have been studied in the literature for the heteronuclear ions of the astrophysical importance, like HeH⁺, LiH⁺, CH⁺, and others. For the plasmas of rare gas mixtures of the role of such processes, on the contrary, is yet to be established.

We study the collisions of heteronuclear molecular and quasimolecular ions with electrons which are accompanied by the charge transfer excitations. Depending on the whether the ion in the initial or the final channels is in a discrete or a continuum state, we distinguish the processes of the electron-impact excitation (bound –bound), dissociative excitation (bound –free), electron-impact association (free –bound) or charge transfer induced by electron impact (free –free). The processes are described on a unified ground using an original semiquantitative theoretical approach [2,3] based on the theory of the nonadiabatic transitions in B + A⁺ + e system and the quasicontinuum approximation for the rovibrational states of the molecular ion. The cross sections and rate constants of the processes above were calculated for ArXe⁺, KrXe⁺, NeXe⁺, NeAr⁺, NeKr⁺, and NeAr⁺ ions which have rather different binding energies, under conditions typical of the active media of the plasma-based radiation sources and dielectric-barrier discharges. We show that the processes studied may have high efficiencies at the incident electron energies of a few electron-volts. The rate constants and cross-sections often exceed those of the processes commonly considered in the kinetic models of the rare gas mixture plasmas. The roles of the specific channels of the electron-impact charge transfer excitation reaction strongly depend on the dissociation energy of a molecular ion, on the structure of its potential energy curves of the initial and final electronic states, and on the gas and electron temperatures of the plasma. We highlight the features of the reactions studies resulting from the small binding energy of the heteronuclear ions considered. The results obtained clearly indicate that the resonant charge transfer excitation processes in the collisions of heteronuclear molecular cations with electrons should be included in the kinetic models of the radiation sources based on the plasmas of noble gas mixtures.

References

1. Y. Tanaka, K. Yoshino, D. E. Freeman, *J. Chem. Phys.* **62**, 4484, (1975).
2. A. Narits, K. Kislov, V. Lebedev, *Atoms* **11**, 60, (2023).
3. A. Narits, K. Kislov, V. Lebedev, *Atoms* **12**, 67, (2024).

#A40: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Photoionization of neutral PAHs in space - New lab data on photoelectric heating

Helgi Rafn Hrodmarsson¹; Gustavo Garcia²; Laurent Nahon²; Emmanuel Dartois³; Thomas Pino³; Philippe Bréchnignac³; Laurent Verstraete⁴

¹ CNRS, LISA UMR 7583, Université Paris-Est Créteil & Université Paris Cité

² Synchrotron SOLEIL

³ Institut des Sciences Moléculaires d'Orsay, CNRS, Université Paris-Saclay

⁴ Institut d'Astrophysique Spatiale (IAS), CNRS, Univ. Paris Sud / Université Paris-Saclay

In the interstellar medium (ISM) and circumstellar environments, photoionization or the photoelectric effect emerges as a prevalent phenomenon. In regions exposed to UV photons, either stellar or secondary photons induced by cosmic rays, polycyclic aromatic hydrocarbons (PAHs) liberate electrons through the photoelectric effect, ef-

ficiently contributing to the heating budget of the gas. In contrast to shielded areas, neutral and cationic PAHs can scavenge electrons and retain a significant portion of the cloud's electronic charge. This dual behavior of PAHs not only influences the gas thermal and dynamical behavior but also plays a pivotal role in shaping the chemistry of the environments. We have measured the photoelectron kinetic energy distribution of PAHs of varying sizes, symmetries, and C:H ratios to describe the photoelectron kinetic energy distribution with a law to be implemented in astrophysical photoelectric models that describe gas heating. We used a double-imaging photoelectron photoion coincidence spectrometer coupled with the DESIRS VUV beamline at the SOLEIL synchrotron to record the gas phase spectra of a series of sublimated PAHs with different sizes and structures in the 13 to 20 C atom range. Our data were used in astrophysical dust photoelectric models to describe the PAH charge and gas photoelectric heating in the ISM. We show that although subtle differences between the molecules in our data set arise from individual electronic structures, the photoelectron KED of PAHs of different sizes and symmetry display remarkable similarities. A general law can thus be implemented in sophisticated ISM astrochemical models to describe their photoelectron KED behavior. Our results predict a maximum photoelectric efficiency that is significantly lower than the previous models, implying a lower interstellar gas temperature and emission.

#A41: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electronically resolved excitation in proton collisions with hydrogen molecules

Corey Plowman¹; Liam Scarlett¹; Mark Zammit²; Igor Bray¹; Dmitry Fursa¹

¹ Curtin University

² Los Alamos National Laboratory

When galactic cosmic ray protons propagate through gas clouds in space they collide with atoms and molecules, transferring energy in the process. In order to calculate the photon flux produced as a result of these collisions knowledge of the rovibrationally resolved cross sections for excitation is required [1]. The most prevalent species in these environments is the hydrogen molecule. However, there is currently no data, experimental or theoretical, for electronically resolved excitation in $p+H_2$ collisions, let alone rovibrationally resolved, at keV energies where they are most significant. As a substitute, equivelocity scaling of the available data for electron collisions with H_2 [2] is currently used to estimate the $p+H_2$ cross sections [1]. Without experimental or theoretical data with which to compare there is no way to assess the accuracy of this simple approach and the effect this approximation has on astrophysical models.

We have developed a semi-classical coupled-channel approach to proton collisions with molecular hydrogen to solve this problem. Since the excitation cross section peaks between 10 to 1000 keV we can model the projectile motion as rectilinear, while still treating the electronic dynamics quantum mechanically. Orientationally averaged results are obtained by analytically integrating over the angular coordinates of the internuclear vector [3]. Using the configuration-interaction expansion method developed for the molecular convergent close-coupling (MCCC) approach to electron collisions [2], we are able to generate very accurate fixed-nuclei states for the hydrogen molecule. This enables us to determine electronically resolved cross sections for transitions into the various excited states of H_2 . A sample of the results is shown in the figure for the dipole-allowed transition $X^1\Sigma_g \rightarrow B^1\Sigma_u$ (Lyman band). Comparison of the present calculations with the scaled electron cross sections reveals significant differences both around the centre of the peak (about 70 keV) and at lower energies where the scaled electron data falls to zero, demonstrating incorrect threshold behaviour. In contrast, our ab initio results for protons correctly incorporate the fact that at keV energies all bound

excitation channels are open. This results in a non-negligible cross section for energies less than about 20 keV, compared to the equivelocity electron data.

The present results represent the first data for state-resolved electronic excitations in $p+H_2$ collisions and show that models relying on equivelocity electron cross sections will be underestimating the photon production rate from proton collisions. This is a significant step toward calculating the rovibrationally resolved cross sections for $p+H_2$ collisions that are required for astrophysical modelling.

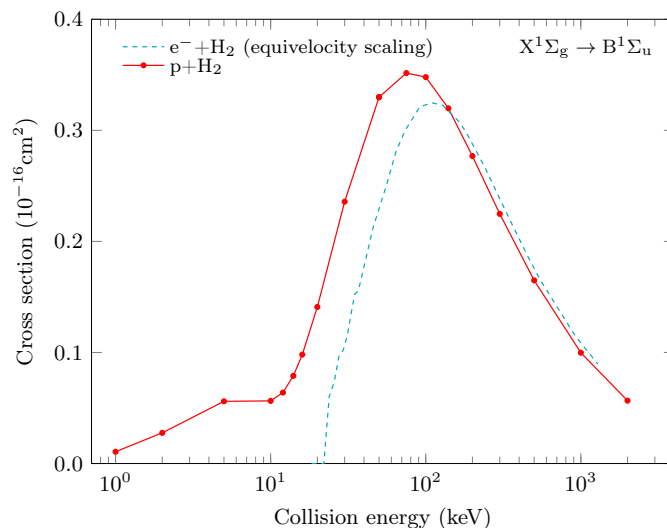


Fig.: Excitation of the $B^1\Sigma_u$ state from the $X^1\Sigma_g$ ground state of H_2 .

[1] M. Padovani et al. *Astron. Astro.* **682**, A131 (2024)

[2] L. H. Scarlett et. al., *Atom. Data Nucl. Data Tables* **137**, 101361 (2021)

[3] I. B. Abdurakhmanov et al. *Phys. Rev. Lett.* **111**, 173201 (2013)

#A42: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Resonances and dissociative dynamics of iron tetracarbonyl acrolein

Sukanta Das¹; Atul Chaudhary²; Hlib Lyshchuk¹; Jaroslav Kočíšek¹; Juraj Fedor¹; Lisa McElwee-White²; Pamir Nag¹

¹ J. Heyrovský Institute of Physical Chemistry of the CAS

² Department of Chemistry, University of Florida

Focused electron beam-induced deposition (FEBID) is a direct-write technique for depositing nanostructures on the surface in the sub-10 nm regime [1]. Due to their magnetic properties, iron nanostructures have the potential to be used in magnetic storage devices, and nano-sensing [2]. For use in FEBID, the iron atoms are surrounded by suitable ligands to ensure the volatility of the precursor. In an ideal situation, after a local irradiation by a focused electron beam, the metal is expected to be deposited and the other fragments should desorb from the surface. However, the resulting structures often have a high amount of contamination coming from the non-metallic fragments. These other fragments are formed by the interaction of precursor with low-energy secondary electrons generated from the interaction of high-energy electron beam (keV) with the substrate. Processes like dissociative ionization (DI), neutral dissociation (ND), and dissociative electron attachment (DEA) break the parent molecule. To improve the purity of the deposited iron, different types of precursor molecules are used

[3, 4] or are still in the developed. Before using compound as a FEBID precursor, it is essential to characterize its dissociation induced by low-energy electrons.

We used the CLUB (CLUSTER Beam) and TEM-QMS (Trochoidal Electron Monochromator) setups [4] to study the fragmentation pattern of a newly synthesised precursor molecule, iron tetracarbonyl acrolein ($\text{Fe}(\text{CO})_4\text{-C}_3\text{H}_4\text{O}$) via DI and DEA processes. At 70 eV incident electron energy (CLUB setup), the presence of the parent cation (mass 224) is negligible. The fragments with m/z (mass to charge) ratios 84 and 112 have the highest abundance. When the data is accumulated over 5–80 eV electron energy range, m/z 56 becomes the most dominating fragment followed by 84 and 112. For the negative ions, which are mostly formed by resonant processes, we did the measurement on the TEM-QMS setup which has a better resolution, it shows the m/z 196 and 168 are present close to 0 eV and have a very narrow spread of 0.5 eV, whereas the other fragments are mostly present for electron energy above 2 eV and have a broad distribution. Using the DFT, we have calculated the thresholds for different fragmentation channels. We discuss possible mechanisms that can lead to the observed fragmentation patterns.

Reference

- [1] Huth et al., O. V. Microelectron. Eng. 2018, 185–186, 9–28.
- [2] Fernández-Pacheco et al., O. V. Materials 2020, 13, 3774.
- [3] Boeckers et al. P. Beilstein J. Nanotechnol. 2024, 15, 500–516.
- [4] Lyshchuk et al. P. Beilstein J. Nanotechnol. 2024, 15, 797–807.

#A43: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Hydrogen Sticking Dynamics on Graphene

Mukul Dhiman¹; Sabine Morriset²

¹ MSME University Gustav Eiffel, Paris

² ISMO University Paris saclay CNRS France

We have performed a full sticking dynamics of H atom on graphenic surface using mixed quantum classical dynamics. These dynamics calculations are parametrized using DFT-VdW-rvv10 functional to obtain potential and phonon modes.

Using this dynamics, for the first time, we have shown the H atom being chemisorbed and physisorbed at the same time.

In the astrophysical context, our results show that at grain temperature of 10K and small initial energy of H atom, the H atom is predominantly physisorbed in the $v = 1$ vibrational state.

#A44: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Source of negatively charged ions for matter-antimatter interaction experiments

Łukasz Kłosowski¹; Mariusz Piwinski²

¹ Nicolaus Copernicus University in Toruń

² Nicolaus Copernicus University in Toruń

Antiprotonic atoms are exotic objects where one or more electrons have been replaced by antiprotons [1]. Numerous phenomena can be observed using such atoms, making them very interesting objects for experimental and theoretical studies. Creating such objects requires

an efficient source of antiprotons, such as the ELENA ring at CERN [2]. The delivered antiprotons can be captured and stored in a Penning trap, part of CERN's AEGIS apparatus [3]. Some atoms with the same electric charge sign (negative in this case) should be stored in the same trapping potential to prepare antiprotonic atoms. After further photo-detachment of electrons from such an ion, the atom and the antiproton may collide to form an antiprotonic atom.

A long-lasting, efficient source of atomic anions is necessary to achieve this goal. The presented system is based on a well-known phenomenon of electron dissociative attachment in electron-molecule collisions [4]. The created anions are stored and cooled inside a multicenter linear Paul trap and then, on request, injected into the Penning trap containing the antiprotons. Such a device was designed, constructed, calibrated and tested at the Nicolaus Copernicus University in Toruń. In the presentation, the source design and preliminary testing results will be discussed.

1. G. Backenstoss "Antiprotonic Atoms" Contemporary Physics 30 (1989) 433–448
2. <https://home.cern/science/accelerators/antiproton-decelerator>
3. <https://aegis.web.cern.ch/index.php>
4. I. Fabrikant et al. "Recent Progress in Dissociative Electron Attachment: From Diatomics to Biomolecules" Advances In Atomic, Molecular, and Optical Physics (2017) 545–657

#A45: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Impact parameter and kinematic information for differential ionization of argon by positron and electron impacts

Karoly Tokesi¹; R.D. DuBois²

¹ HUN-REN Institute for Nuclear Research

² Missouri University of Science and Technology, Rolla MO 65409 USA

We present ionization cross sections in collisions between electron and positron impact with Ar(3p) target. The calculations were performed classically using the three body CTMC approximation. We found that the ionization probabilities as a function of impact parameter show different distributions for electron and positron impact. For the case of positron impact the distribution is symmetric, for the case of electron impact the distribution is asymmetric. Furthermore we found that the dominant part of ionization occurs for impact parameters smaller than the 3p radius.

Acknowledgments

The work was supported by the Bilateral relationships between Qatar and Hungary in science and technology (S&T) under the project number 2021-1.2.4-TÉT-2021-00037.

References

- [1] R.D. DuBois and K. Tőkési, Atoms 11 51 (2023)

#A46: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Commissioning of the Transverse Free-Electron Target at the Heavy-Ion Storage Ring CRYRING@ESR

Alexander Borovik¹; Carsten Brandau²;
Michel Döhring³; A. Gumberidze⁴; Anton Kalinin²; Arya Krishnan⁵; Dariusz Banaś⁶; Elena O. Hanu⁷; Esther Babette Menz²; Jan Glorius⁴; Johannes Viehmann⁸; K. Szary⁹; Michael Lestinsky²; Mirko Looshorn¹⁰; Pawel Jagodzinski¹¹; Pierre-Michel Hillenbrand²; Rohit Tyagi¹²; Shuxing Wang¹; Stefan Schippers¹³; Uwe Spillmann²

¹ I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

² GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

³ JLU Gießen

⁴ GSI Helmholtzzentrum für Schwerionenforschung

⁵ GSI, Institute for Applied Physics, Technische Universität Darmstadt, Darmstadt

⁶ Institute of Physics, Jan Kochanowski University, 25-406 Kielce, Poland

⁷ GSI, Uni Frankfurt, HI Jena

⁸ Universität Kassel

⁹ Institute of Physics, Jan Kochanowski University

¹⁰ Uni Gießen, Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Gesellschaft für Schwerionenforschung, Campus Gießen

¹¹ Jan Kochanowski University, Kielce and Central Office of Measures, Warszawa

¹² University of Kassel

¹³ Justus-Liebig-Universität Gießen, I. Physikalisches Institut

Electron-ion collision experiments in a merged beams geometry (electron cooler) are well established at ion storage rings. A complete new range of experiments is possible if the geometry is changed to a crossed-beams setup in 90° angle between the electron and ion beams employing a dedicated free-electron target. The target bridges the gap between low-collision-energy experiments in electron coolers and those employing quasi-free electrons of gas-jet targets. Compared to the latter, the absence of a target nucleus enables unambiguous studies of processes, which are otherwise masked by competing reactions with the target nucleus. As compared to an electron cooler, the interaction region of a transverse target is spatially well localized. This facilitates X-ray and electron spectroscopy with relatively large solid angles. Over the last years, a specially tailored electron-target for heavy-ion storage rings was developed and built at the University of Giessen in cooperation with GSI. Its scientific prospects have been outlined in the CRYRING@ESR Physics Book [1].

The project benefits from decades-long experience of single-pass electron-ion-collision experiments [2-4]. The target is equipped with a versatile electron gun that is optimized for an operation in storage rings. The electron gun can be fully retracted from the storage ring to a position behind a gate valve. One of the specific design criteria was a rather large opening for the ion beam in order to accommodate ion injection into the storage ring on different orbits. First electron-ion beam experiments showed that in total only up to 20

The electron target creates a ribbon-shaped high-intensity electron beam with energies up to 12.5-keV (lab system).

The multi-electrode assembly offers a decoupling of electron energy and electron density, which is beneficial for the ultra-high vacuum conditions in the ring. It also offers a quasi-constant electron density over large energy ranges. We report on the latest achievements during the commissioning beamtimes of the electron target at the CRYRING@ESR. The evaluation of the performance and operation behaviour is ongoing.

This research was supported by the ErUM-FSP APPA (BMBF grant nos. 05P15RGFAA, 05P19RGFA1, 05P21RGFA1, 05P24RG2),

<https://fsp-appa.fair-center.eu>.

References

- [1] Lestinsky M et al. 2016 Eur. Phys. J Spec. Top. 225 797
- [2] Ebinger B et al. 2017 Nucl. Instrum. Methods B 408 317
- [3] Jin F et al. 2024 Eur. Phys. J. D 78 68
- [4] Döhring B M et al. 2025 Atoms 13(2) 14

#A47: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Associative ionisation of $H(1s) + H(ns)$: a semi-classical description

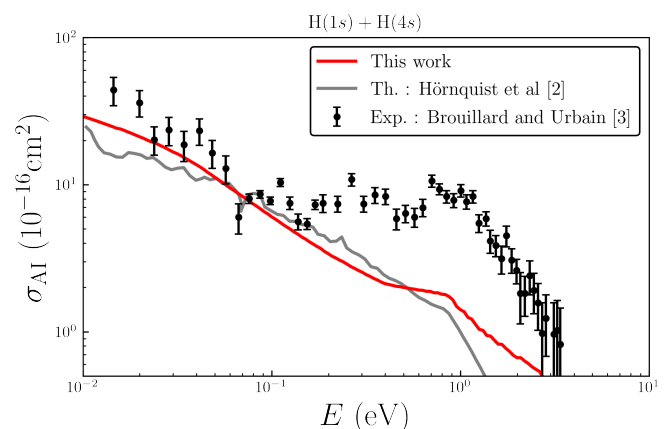
Pierre GUICHARD¹; Xavier Urbain²; Paul-Antoine Hervieux³

¹ Université de Strasbourg

² Université catholique de Louvain

³ Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg

Associative ionisation (AI), a fundamental atomic collision process, plays a crucial role in atomic physics, plasma physics and astrophysics, contributing to the ionisation of atoms and the formation of molecules. In this work we study AI in low-energy hydrogen atom collisions, in particular the reaction $H(1s) + H(ns) \rightarrow H_2^+ + e^-$ with $2 \leq n \leq 10$, using a semi-classical approach. We extend the Duman-Shmatov-Mihajlov-Janev (DSMJ) model [1] to include short-range interactions and multistate transitions, thereby improving the predictive capabilities for low-energy AI processes. While the approach in [2] provided valuable insights, it relied on highly sophisticated quantum mechanical calculations and is therefore limited to collisions with $n \leq 4$. In contrast, our semi-classical model reproduces the results of [2] very well at significantly lower computational cost and gives a better intuition of the underlying physical processes, making it a more efficient alternative while remaining in good agreement with the experimental data [3] (see figure). This work not only aims at reproducing these results, but has also been used to explore the regime with $n \gg 1$.



[1] R. K. Janev and A. A. Mihajlov, Excitation and de-excitation processes in slow collisions of Rydberg atoms with ground-state parent atoms, Physical Review A 20, 1890–1904 (1979).

[2] J. Hörnquist et al, Associative ionization in collisions of $H^+ + H^-$ and $H(1s) + H(ns)$, Physical Review A 108, 052811 (2023).

[3] F. Brouillard and X. Urbain, Associative Ionisation in Low Energy Collisions, Phys. Scr. T96, 86 (2002).

#A48: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Crossed-beam Scattering Dynamics of Atomic Nitrogen Ions with Carbon Dioxide Molecules

Jerin Judy; Dasarath Swaraj; Fabio Zappa; Roland Wester

Universität Innsbruck

Crossed molecular beam experiments serve as a robust approach for investigating the dynamics of elementary gas-phase reactions [1], with Velocity Map Imaging (VMI) enabling the determination of energy and angle-resolved differential cross-sections [2]. Building on our previous investigation of the reactive scattering between N^+ ions and O_2 neutrals, where two distinct product channels were identified and characterized [3]—we now report the first differential cross-section measurements for the $N^+ + CO_2$ reaction, resolved in both energy and angle, over a collision energy range of 0.16 eV to 1.52 eV. Two primary reaction pathways are observed: charge transfer and dissociative charge transfer. For each channel, we quantify the branching ratios and present velocity map images from which the internal energy distributions and angular scattering patterns of the products are extracted. These experimental findings provide critical data for benchmarking theoretical models and emphasize the necessity of further theoretical work to elucidate the underlying mechanisms governing ion-molecule interactions.

References

- [1] N. Balucani, G. Capozza, F. Leonari, E. Segoloni, and P. Casavecchia Int. Rev. Phys. Chem. 25, 109 (2006)
- [2] R. Wester Phys. Chem. Chem. Phys. 16, 396 (2014)
- [3] D. Swaraj, J. Judy, F. Zappa, R. Wester Phys. Scr. 100, 025408 (2025)

#A49: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electron and Ion Induced Reactions with Chlorpyrifos Molecules

Alexandra Jančíšínová; Navya Arepalli; Peter Papp; Stefan Matejcik

Department of Experimental Physics, Comenius university, Bratislava, Slovakia

Abstract: Chlorpyrifos (O,O-diethyl O-3,5,6-trichloro-2-pyridyl phosphorothioate) is one of the harmful pesticide that persist long time in the environment and effect human health. As a result of its accumulation in the environment and the effect it causes on human health its degradation into non-harmful substances is of high importance. In recent days, Plasma assisted degradation that involves highly energetic species such as radicals, ions to induce molecular fragmentation is emerging as an effective method for their removal. In this work, Density Functional Theory (DFT) based calculations were performed to investigate the various degradation pathways of chlorpyrifos. Potential protonation sites were identified through the Natural Bond Orbital (NBO) analysis, charge distribution, electrostatic potential (ESP) mapping and the calculation of proton affinities at various sites. In order to predict the bonds that are most likely to break under plasma conditions, Bond dissociation energies (BDEs) of different bonds have been calculated. Along with the Plasma degradation pathways, Time-Dependent Density Functional Theory (TD-DFT) was also performed to understand the photo-induced electronic transitions and excited-state pathways that facilitate degradation. This theoretical study explains the plasma induced degradation of chlorpyrifos at molecular

level, helping to design better ways for the pesticide removal using plasma technologies.

References

- [1] E. Taillebois et al. "Molecular features and toxicological properties of four common pesticides, acetamiprid, deltamethrin, chlorpyrifos and fipronil". *Bioorganic & Medicinal Chemistry*, 23 (2015) 1540–1550
- [2] Quintano, M.M., Rocha, W.R. "Computational insights into the reactivity of chlorpyrifos and chlorpyrifos-methyl toward singlet oxygen". *Journal of Molecular Modeling*, 27, 282 (2021).

Acknowledgement

This work was supported by the Slovak Research and Development Agency under the Contract no. APVV-22-0522 and the Slovak Grant Agency for Science (contract no. VEGA 1/0553/22). Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I01-03-V04-00047. This work was supported in part through the Comenius University in Bratislava CLARA@UNIBA.SK high-performance computing facilities, services and staff expertise of Centre for Information Technology (<https://uniba.sk/en/HPC-Clara>).

#A50: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Dissociative positronium attachment in halogen gases

Robyn Wilde¹; Gleb Gribakin²; Ilya Fabrikant³

¹ Oregon Institute of Technology

² Queen's University Belfast

³ University of Nebraska, Lincoln

We calculate the cross section and the rate constant for the process of dissociative positronium attachment to the F_2 molecule at thermal energies. The process results in an anomalously large positronium annihilation rate, which can possibly explain the observed rapid positronium annihilation in halogen gases.

When fast positrons (e.g., those produced in β^+ decay) thermalise and ultimately annihilate in matter, a sizeable fraction of them forms positronium (Ps) [1,2]. Its formation is typically statistical, with 25% of it being para-Ps (p -Ps, total spin $S = 0$), and 75% being ortho-Ps (o -Ps, $S = 1$). In vacuum, they annihilate predominantly by 2γ (p -Ps) and 3γ (o -Ps) annihilation, with the lifetimes of 0.125 and 142 ns, respectively. In gases and condensed-matter systems, the lifetime of o -Ps is usually reduced by its interaction with surrounding molecules or surfaces.

The o -Ps annihilation rate due to collisions with gas molecules is written as $\lambda = 4\pi r_0^2 cn^1 Z_{\text{eff}}$, where n is the gas density and $4\pi r_0^2 cn$ is the Dirac rate for singlet positron annihilation in a gas of electrons. The measured values of the parameter $^1Z_{\text{eff}}$ are quite small for most molecular gases, $^1Z_{\text{eff}} \sim 1$. By contrast, o -Ps annihilation in several molecular gases yields much larger $^1Z_{\text{eff}}$ values. In particular, $^1Z_{\text{eff}} = 1.15 \times 10^4$ and 1.26×10^4 for Br_2 and I_2 , respectively [3]. We suggest that these high $^1Z_{\text{eff}}$ values are due to the process of dissociative Ps attachment, $Ps + X_2 \rightarrow PsX + X$, where X stands for a halogen atom. This process is similar to the dissociative electron attachment which leads to the formation of negative ions.

We calculate the cross section and rate of this process for the F_2 molecule for which the process is exothermic, and therefore can occur at room temperature. We start with the Ps- F_2 scattering calculations which take into account electron exchange and correlations within the framework of the free-electron-gas model [4]. The calculations reveal several resonances. Similar to the process of dissociative electron attachment, a Σ_u resonance contributes to the dissociative Ps attachment at thermal energies. We determine the resonance position and width as functions of the internuclear separation, and

use them as inputs for the local version of the quasiclassical theory of dissociative attachment [5]. Our calculations yield the rate constant $\alpha = 0.19 \times 10^{-10} \text{ cm}^3/\text{s}$, which corresponds to $Z_{\text{eff}} \sim 10^3$. This value is anomalously large and is only one order of magnitude lower than those for Br_2 and I_2 .

- [1] M. Charlton, Rep. Prog. Phys. **48**, 737 (1985).
- [2] P. J. Schultz and K. G. Lynn, Rev. Mod. Phys. **60**, 701 (1988).
- [3] K. Wada *et al.*, Eur. Phys. J. D **66**, 108 (2012).
- [4] I. I. Fabrikant and R. S. Wilde, Phys. Rev. A **97**, 052707 (2018).
- [5] A. K. Kazansky and I. S. Yelets, J. Phys. B: At. Mol. Phys. **17**, 4767 (1984).

#A51: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Gas phase collisions of O^+ ions in ^4S and ^2D states with molecular moieties of space-relevant polymers

Christian Alcaraz¹; Cintia Aparecida Pires Da Costa²;
Daniela Ascenzi²; Matteo Michielan²; Nandana
Pattathadathil²; Nicolas Solem¹; Roland Thissen¹

¹ Université Paris-Saclay, CNRS, Institut de Chimie Physique

² Department of Physics, Università di Trento

Organic polymers have wide applications in the aerospace industry (e.g. in satellites and spacecrafts). However, when such materials are used in spacecraft external surfaces in Low Earth Orbit (LEO - up to 2000 km above Earth's surface), they are subject to erosion due to exposure to the main atmospheric components at such altitudes, i.e. atomic oxygen (AO) and O^+ ion. Current strategies to limit polymer degradation (e.g. coatings and self-modifying materials) are largely based on a trial-and-error approach, due to a lack of understanding of the reaction mechanisms responsible for erosion.

Atomic oxygen in ionized form (O^+) is the dominant cation in the Earth's thermosphere, where it is known to exist not only in its ground state (^4S) but also in its excited states ^2D and ^2P . Due to their long lifetimes (3.6 hours for ^2D , 4.6 s for ^2P) they have sufficient time to react before de-excitation under the low-pressure conditions of LEO. Hence, performing single collision gas-phase experiments between state selected O^+ ions and polymers will permit to gain insight into the erosion mechanisms at an atomistic level, by identifying molecular sites most vulnerable to O^+ attack. Due to the low volatility of the monomers, we identify key molecular moieties of space-grade polymers that are volatile enough to be brought to the gas phase, while retaining the relevant functional groups and molecular structures of the whole polymers. In particular we choose: a) benzene (C_6H_6), naphthalene (C_{10}H_8) and phenanthrene ($\text{C}_{14}\text{H}_{10}$), as templates for graphite; b) ethylbenzene ($\text{C}_6\text{H}_5\text{CH}_2\text{CH}_3$), styrene ($\text{C}_6\text{H}_5\text{CHCH}_2$) and 1,3-diphenylpropane ($\text{C}_6\text{H}_5(\text{CH}_2)_3\text{C}_6\text{H}_5$), as templates for polystyrene c) diphenylether ($\text{C}_6\text{H}_5\text{OC}_6\text{H}_5$), N-methylmaleimide ($\text{CH}_3\text{-NCOCHCHCO}$) and N-vinylformamide (HCONHCHCH_2) as templates for Kapton. In addition, aniline and phenol are used in substitution of 4-aminophenol.

Experiments are conducted using the CERISES setup: a guided ion beam tandem mass spectrometer that couples ion generation via tunable VUV light (from the DESIRS beamline of the SOLEIL synchrotron radiation facility) with octupolar RF guiding and trapping of ions to measure absolute integral reactive cross sections and product branching ratios as a function of collision energy (ranging from meV to tens of eV).

The selective generation of O^+ ions in the ground (^4S) is achieved via dissociative photoionization of O_2 at 19.4 eV photon energy, while a

mixture of ground and first excited (^2D) state is produced at 23.05 eV photon energy. In the latter case, a "titration" method is put in place to estimate the relative yield of ^4S and ^2D states by comparing results on the reactivity of O^+ with CD_4 with reference data obtained using a state-selective method (PEPICO) [1].

Absolute cross sections and branching ratios for the reactions of state selected O^+ ions will be presented for a selection of the above mentioned molecules. In most cases the main reactivity is due to dissociative and non dissociative charge exchange. This study will improve our understanding of polymer erosion in space and aid the design of more resilient materials for satellites, space stations, and spacecraft.

[1] B. Cunha de Miranda, C. Romanzin, S. Chefdeville *et al.*, J. Phys. Chem. A, 2015, 119(23): 6082–98

Acknowledgments

The research is carried out within the National Recovery and Resilience Plan (NRRP), Mission 4, Component 2, Investment 1.1, Call for tender No. 1409 (14.9.2022) by the Italian Ministry of University and Research (MUR), funded by the European Union –NextGenerationEU –Project Title P20223H8CK "Degradation of space-technology polymers by thermospheric oxygen atoms and ions: an exploration of the reaction mechanisms at an atomistic level" - CUP E53D23015560001. Thanks to Laurent Nahon & DESIRS team @SOLEIL SRF for assistance under Proposal No. 20240422.

#A52: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

C_{60}^+ collisions with low-energy electrons at the Cryogenic Storage Ring

Lucia Enzmann¹; Jonas Bechtel¹; Bhalchandra Sitaram
Choudhari¹; Manfred Grieser¹; Florian Grussie¹; Leonard
Isberner²; Claude Krantz³; Holger Kreckel¹; Stefan
Schippers²; Viviane Schmidt¹; Andreas Wolf¹; Oldřich
Novotný¹

¹ Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

² I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Gießen, Germany

³ GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

The absorption spectrum of diffuse interstellar clouds displays a rich set of lines - the diffuse interstellar bands (DIBs). The origin of the DIBs is intensely investigated since their first observation in 1922 [1] and remains elusive even today. Already with the discovery of C_{60} , Kroto *et al.* [2] proposed C_{60} as a possible carrier for the DIBs. This hypothesis was later confirmed by laboratory studies, which assigned the first DIBs to C_{60}^+ [3]. Further evidence from laboratory investigations and observational studies using the Hubble Space Telescope has strengthened confidence in the existence of C_{60}^+ in the interstellar medium (ISM) and its contribution to the DIBs. However, the origin and destruction pathways of C_{60}^+ in the ISM remain a puzzle. For this, reaction kinetic data is needed to model the C_{60}^+ chemistry. Obtaining laboratory data with astrophysical relevance requires experimental conditions comparable to those in the ISM, such as low temperatures and intermediate densities [4].

The electrostatic Cryogenic Storage Ring (CSR) [5] at the Max Planck Institute for Nuclear Physics in Heidelberg is a suitable experimental environment to mimic the cold ISM, since it reaches vacuum chamber temperatures of < 10 K. In the electron-ion merged-beams setup, the stored ion beam is overlapped with a low-temperature electron beam produced by a photocathode [6], and electron-ion collisions can be studied at well-defined and tunable collision energies. We stored C_{60}^+

ions in the CSR and studied electron collisions at collision energies between few meV and ~ 85 eV. Long ion beam storage times of up to 500 s allowed to investigate the reaction dynamics for an evolving internal excitation of the stored C_{60}^+ ions. We observed various collisional processes such as recombination, ionization, fragmentation and fragmentation-ionization. In comparison to collisions of smaller ionized molecules with electrons, C_{60}^+ shows a different recombination behavior. In the same way, we studied interactions of C_{70}^+ with free electrons. Future electron-ion collision experiments that are planned at the CSR include measurements of other DIB carrier candidates, for example Polycyclic Aromatic Hydrocarbons. Additionally, recombination experiments with smaller fullerene species are considered.

[1] Heger, M. L., Lick Observatory Bulletin 10, no. 337, pp. 146-147 (1922)

[2] Kroto, H., Heath, J., O'Brien, S. et al., Nature 318, pp. 162-163 (1985)

[3] Campbell, E., Holz, M., Gerlich, D. et al., Nature 523, pp. 322-323 (2015)

[4] Herbst, E. and van Dishoeck, E.F., Annual Review of Astr. and Astroph. 47, pp. 427-480 (2009)

[5] von Hahn, R. et al., Rev. Sci. Instrum. 87, 063115 (2016)

[6] Shornikov, A. et al., Phys. Rev. ST Accel. Beams 17, 042802 (2014)

#A53: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Convergent Close-Coupling Approach to Electron-Impact Dissociative Excitation and Ionisation of H_3^+

Reese Horton¹; Michael Pak²; Igor Bray¹; Dmitry Fursa¹

¹ Curtin University

² Air Force Institute of Technology

The results of a newly developed version of the Molecular Convergent Close-Coupling (MCCC) method [1,2] of calculating cross sections for electron scattering on the H_3^+ molecule are reported. Integrated cross sections for dissociative electronic excitation and ionisation are presented, yielding good agreement with the experiment [3,4]. The causes of previous disagreements between theory and experiment are identified. The method is presented in both the fixed-nuclei and adiabatic nuclei formulations, with optional point-group symmetry adaptation. The results of the first-ever calculation of fragment kinetic energy release distributions in electron impact dissociation of H_3^+ are also reported, yielding good agreement with the strong textexperiment at high energies. The new method opens the door to the modelling of electron and positron scattering on polyatomic molecules using CCC techniques.

Fig.: Comparison of the total dissociative excitation cross section for electron scattering on H_3^+ and D_3^+ in several MCCC models [1,2] with the experiments of Lecointre et al [3], Jensen et al [4], the R-matrix calculation of Gorfinkel and Tennyson [5] and the complex-Kohn calculation of Orel [6].

[1] Horton et al, Phys. Rev. Lett. **134**, 063001 (2025).

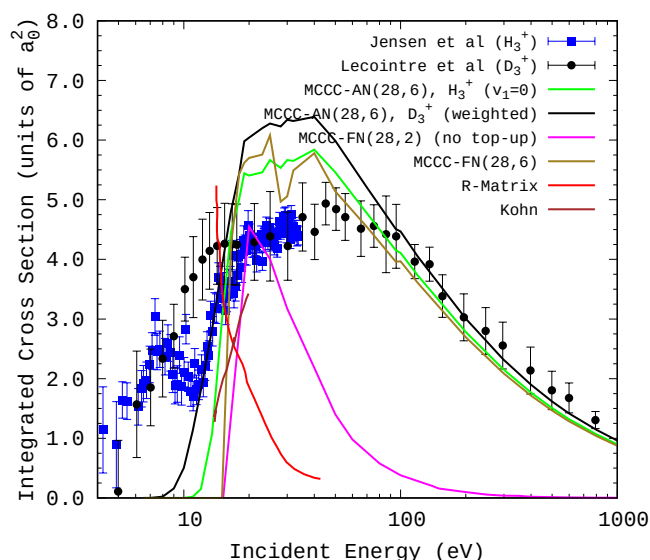
[2] Horton et al, Phys. Rev. A. **111**, 022802 (2025).

[3] Lecointre et al, J. Phys. B. **42**, 075201 (2009).

[4] Jensen et al, Phys. Rev. A. **63**, 052701 (2001).

[5] Gorfinkel and Tennyson, J. Phys. B **38**, 1607 (2005).

[6] Orel, Phys. Rev. A. **46**, 1333 (1992).



#A54: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

From megabarns to attoseconds: How to relate the cross-section with the time delay

Anatoli Kheifets¹; JiaBao Ji²; Kiyoshi Ueda³; Meng Han⁴; Hans Jakob Wörner²

¹ Australian National University

² ETH Zürich

³ Tohoku University

⁴ Kansas State University,

Traditionally, photoionization studies have been carried out in the frequency domain by measuring the cross-section and angular distributions of photoelectrons. Newly developed laser assisted interferometric techniques expand these studies into the time domain thus marking the advent of attosecond science [1]. Here we show that the attosecond time delay, also known as the Wigner time delay [2], can be retrieved from the photoionization cross-section by way of the logarithmic Hilbert transform (LHT). The LHT can be used to relate the cross-section and time delay in a large number of single-photon resonant ionization processes. It provides a good estimate of time delay near atomic and molecular shape resonances [3], confinement resonances in the endohedrally trapped Xe@C₆₀ and the Cooper minima in the valence shells of noble gas atoms [4]. Fano resonances can also be treated in the similar way. Particularly interesting is application of the LHT to two-photon XUV+IR ionization where the Fano resonance appears in one of the two interfering channels of the RABBITT process [5].

[1] P.B. Corkum and F. Krausz, Nat. Phys. **3**, 381 (2007).

[2] A.S. Kheifets, J. Phys. B **56**, 022001 (2023)

[3] A.S. Kheifets and S. Catsamas, Phys. Rev. A **107**, L021102 (2023)

[4] Jia-Bao Ji et al., New J. Phys. **26**, 093014 (2024)

[5] A.S. Kheifets, arXiv preprint 2410.16696 (2024)

#A55: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Spin and Orbital Angular Momentum in Attosecond Pulses of Light

Alba de las Heras¹; David Schmidt²; Julio San Román³; Javier Serrano³; Jonathan Barolak²; Bojana Ivanic²; Cameron Clarke²; Nathaniel Westlake²; Daniel E. Adams²; Luis Plaja³; Charles G. Durfee²; Carlos Hernández-García³

¹ Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science

² Colorado School of Mines

³ Universidad de Salamanca

We theoretically and experimentally demonstrate the generation of attosecond vortex pulse trains, i.e. a succession of attosecond pulses with a helical wavefront, resulting from the coherent superposition of a comb of high-order harmonics carrying the same orbital angular momentum (OAM)[1]. The control of spin and OAM degrees of freedom in extreme ultraviolet attosecond pulses brings new capabilities to spectroscopic and imaging applications in chiral and magnetic systems.

[1] A. de las Heras et al. *Optica*, 11, 1085 (2024)

#A56: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Amplification of spontaneous emission from doubly excited He atoms

Janez Turnšek¹; Š. Krušič¹; A. Mihelič¹; K. Bučar¹; L. Foglia²; R. Mincigrucchi²; M. Krstulović²; M. Coreno²; K.C. Prince²; C. Callegari²; A. Benediktovitch³; R. Osellame⁴; C. Vozzi⁴; R. Martinez Vazquez⁴; A.G. Ciriolo⁴; E. Principi²; M. Žitnik¹

¹ J. Stefan Institute

² Elettra-Sincrotrone Trieste

³ Deutsches Elektronen-Synchrotron

⁴ Institute for Photonics and Nanotechnologies,

We have detected self-amplified spontaneous emission (ASE) from He atoms in $3^+ 1P^o$ doubly excited state. This resonance with 63.66 eV excitation energy autoionizes within 80 fs but may also decay by spontaneously emitting a 40.75-eV photon to populate the $1s3s$ $1S^e$ atomic state with 3×10^{-4} probability [1,2]. Despite such a small fluorescence branching ratio, our recent calculations in the paraxial approximation predicted strong ASE in the forward direction if a sufficiently dense and long column of helium gas is traversed by intense, resonantly tuned XUV light [3]. Indeed, stimulated amplification of the weak $3^+ 1P^o \rightarrow 1s3s 1S^e$ fluorescence decay was observed at the EIS-TIMEX beamline using light pulses from the free electron laser (FEL-1) facility FERMI in Trieste, Italy. The helium gas column was a few mm long and the pressure went up to 100 mbar. The 50-fs long FEL pulses with few tens of μJ energy were focused to the $15 \times 26 \mu m^2$ cross section in the center of an open-end glass micro-capillary. A maximum observed average conversion factor from the number of probe photons to the number of ASE photons was 4.1%, quite consistent with the theoretical prediction. Simultaneously with ASE, we have measured position-resolved VIS emission spectra collecting the light from different positions along

the gas cell. The VIS signal was due to late transitions between singlet and triplet singly excited states in the atomic He, as well between the excited states in He+ ions. The intensity of VIS lines was found to diminish with a distance from the cell entrance as dictated by absorption of the FEL light along the cell. A weak correlation of the single-shot VIS spectra with the ASE emission was detected.

[1] F. Penent et al., *Phys. Rev. Lett.* 86, 2758-2761 (2001).

[2] J. Soderstrom, *Phys. Rev. A* 77, 012513 (2008).

[3] Š. Krušič et al., *Phys. Rev. A* 107, 013113-1-13 (2023).

#A57: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Adiabatic alignment of alkali dimers on the surface of helium nanodroplets

Emil Hansen; Lorenz Kranabetter; Henrik H. Kristensen; Nicolaj K. Jyde; Henrik Stapelfeldt

Aarhus University

Moderately intense laser pulses can confine the axes of molecules to axes that are fixed in space through the polarizability interaction. This process is termed laser-induced alignment. [1,2] A large number of studies have established that a key parameter for achieving a high degree of alignment is a low rotational temperature of the molecules explored. For samples of gas phase molecules, a low temperature is typically achieved using supersonic molecular beams and, in special cases, through selection of a single or a few rotational quantum states by electrostatic deflection or focusing. The rotational temperature can also be lowered by embedding molecules in He nanodroplets inside which molecules are still exhibiting free rotation. A series of studies showed that the 0.37 K temperature of molecules in He nanodroplets makes it possible to obtain very high degrees of alignment in the adiabatic limit where the alignment pulse is turned on and off slowly as compared to the rotational period of the molecules [3,4]. Most molecules are located inside He droplets but some species, in particular dimers and trimers of alkali metal atoms are bound at the surface of the droplets. In this work, I present the first results on adiabatic laser-induced alignment of alkali dimers on He droplet surfaces complement to recent studies of nonadiabatic alignment [5,6].

The He droplets, consisting of about 12000 He atoms are doped with alkali atoms, which leads to the formation of alkali dimers in either the electronic ground state $1\Sigma_g^+$ or the lowest-lying triplet state, $3\Sigma_u^+$. The doped droplets are irradiated by pulses from two laser beams. The first pulse, (~ 200 ps, 1300 nm) is used to align the dimers. The second, delayed probe pulse (~ 50 fs, 800 nm) Coulomb explodes the Ak dimers through multiphoton absorption into a pair of Ak+ ions thanks to its high intensity. The emission directions of the Ak+ fragment ions, detected by a velocity map imaging (VMI) spectrometer backed by a TPX3Cam, allow us to determine the degree of alignment of the alkali dimers at the time the probe pulse arrives.

With this technique, we simultaneously study the alignment dynamics of the Ak dimers in both the $1\Sigma_g^+$ and $3\Sigma_u^+$ states. We obtain degrees of alignment exceeding 0.9 using only moderate ($\sim 10 \text{ GW cm}^{-2}$) alignment pulse intensities in good agreement with numerical calculation based on solution of the time-dependent Schrödinger equation. Furthermore, we find that resonance effects occur in the K₂ and Rb₂ dimers using 1300 nm, leading to dissociation through absorption. Finally, these measurements may provide insight into the rotational temperature of the dimers and the timescales of rotational decoherence and population decay due to coupling between the alkali dimer and the droplet.

[1] H. Stapelfeldt and T. Seideman, *Rev. Mod. Phys.* 75, 543 (2003)

[2] C. P. Koch, M. Lemesko, and D. Sugny, *Rev. Mod. Phys.* 91, 035005 (2019).

[3] B. Shepperson *et al.*, *J. Chem. Phys.* 147, 013946 (2017).

- [4] A. S. Chatterley *et al.*, Nat. Commun. **10**, 133 (2019).
 [5] L. Kranabetter *et al.*, Phys. Rev. Lett. **131**, 053201 (2023)
 [6] H. H. Kristensen *et al.*, arXiv:2502.14521v1 [physics.atm-clus] (2025)

#A58: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Verifying Fano's propensity rules by interfering photoelectron wavepackets of different parities

Nedjma Ouahioune¹; Dominik Hoff²; Praveen Kumar Maroju²; Anne L'Huillier²; Jan Marcus Dahlström²; Mathieu Gisselbrecht²

¹ Department of Physics, Lund University, Lund, Sweden.

² Department of Physics, Lund University, Lund, Sweden

Synopsis High-order Harmonic Generation (HHG) driven by few-cycle near-infrared (NIR) pulses produces a comb of spectrally broad odd harmonics in the eXtreme Ultra-Violet (XUV) range. Owing to the spectral width of the harmonics, electron wave packets (EWPs) singly photoionized to the continuum interfere with EWPs taking a two-photon path (XUV+NIR). We analytically discuss the relationship between these interferences and Fano's propensity rules in helium.

High-order Harmonic Generation (HHG) driven by near-infrared (NIR) pulses generates phase-locked odd-order harmonics of the driving laser frequency in the eXtreme Ultra-Violet (XUV) range. These can be used to produce electron wave packets (EWPs) via photoionization that are separated by twice the NIR energy. In the RABBIT (Reconstruction of Attosecond Beatings By Interference of Two-photon transitions) technique [1], a weak delayed replica of the NIR laser couples the EWPs generated by the consecutive harmonics to the same final energy through the absorption/emission of an additional NIR photon. The resulting interferences exhibit oscillations at twice the NIR frequency and can be used to extract information about the photoionization process.

In this work, we consider RABBIT with few-cycle NIR pulses in helium. Ascribed to the short pulse duration, the harmonics are spectrally broad, allowing EWPs singly photoionized to the continuum by the XUV (1-photon path) to interfere with EWPs that undergo an additional transition by absorbing or emitting a NIR photon (two-photon path). When angular resolution is available, this translates into oscillations at the laser frequency. We propose a link between the modulations and Fano's propensity rules[2,3].

For this, we analytically describe the angular-dependence of the EWP interferences originating from the one-photon/two-photons parity mixing in helium using a partial wave expansion. We show that the odd expansion coefficients h_{2n+1} ($n=0,1$) allow extracting the radial two-photon transition amplitudes from a same intermediate state.

References

- [1] P.M. Paul *et al.*, Science **292**, 1689-1692, (2001)
 [2] D. Busto *et al.*, Phys. Rev. Lett. **123**, 133201, (2019)
 [3] M. Bertolino *et al.*, J. Phys. B: At. Mol. Opt. Phys. **53**, 144002, (2020)

#A59: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Correlated Strong-Field Double Ionization

Susmita Jana¹; Katharina Buczolic¹; Takeshi Sato²; Kenichi L. Ishikawa²; Joachim Burgdörfer¹; Iva Březinová¹

¹ Institute for Theoretical Physics, Vienna University of Technology,

² 1.Department of Nuclear Engineering and Management, Graduate School of Engineering, 2.Research Institute for Photon Science and Laser Technology 3.Photon Science Center, Graduate School of Engineering, The University of Tokyo,

Correlated strong-field double ionization exhibits a characteristic 'knee' structure in the double ionization yield as a function of intensity [1-3]. This feature arises because of the contribution from the nonsequential double ionization (NSDI) process, in which the electron-electron interaction rather than independent tunneling plays a key role.

Generally, NSDI enhancement is attributed to the rescattering of the first ionized electron at the parent ion, thereby transferring the second electron to an easily ionizable excited state or the continuum [4]. However, some experiments have observed an enhancement of NSDI also in elliptically polarized fields, challenging the conventional rescattering picture [5]. Full ab initio calculations of this two-electron problem have remained computationally challenging and, up to now, only a few promising results have become available for He [6]. In the present study, we address the challenge and perform fully correlated calculations of NSDI in strong fields by employing the multiconfigurational time-dependent Hartree-Fock method (MCTDHF) [7] for Be atoms and linearly polarized fields. Because of its low first ionization potential of 9.32 eV, Be is a prime candidate for an ab initio simulation. We utilize the two-particle reduced density matrix [8] and investigate the two-electron dynamics as a function of time and intensity. As the intensity increases, we see signatures of the rescattering process leading to an enhancement in the NSDI yields.

References

- [1] D. N. Fittinghoff *et al.* Phys. Rev. Lett. **69**, 2642–2645 (1992).
 [2] B. Walker *et al.* Phys. Rev. Lett. **73**, 1227–1230 (1994).
 [3] Y. H. Lai *et al.* Phys. Rev. A **101**, 013405 (2020).
 [4] P. B. Corkum. Phys. Rev. Lett. **71**, 1994–1997 (1993).
 [5] G. D. Gillen, M. A. Walker, and L. D. Van Woerkom. Phys. Rev. A **64**, 043413 (2001).
 [6] A. Zielinski, V.P. Majety, A. Scrinzi, Phys. Rev. A **93**, 023406 (2016).
 [7] T. Sato *et al.* Phys. Rev. A **94**, 023405 (2016).
 [8] F. Lackner *et al.* Phys. Rev. A **95**, 033414 (2017).

#A60: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Effect of Laser Repetition Rate on Electron Emission from Tungsten Nanotip

Haritha Venugopal¹; Abhisek Sinha¹; Sanket Sen¹; Ram Gopal²; Vandana Sharma¹

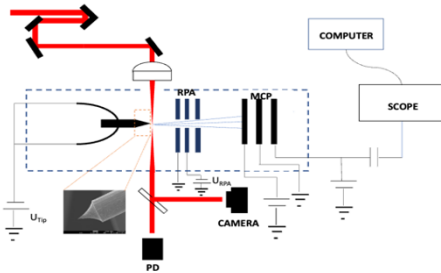
¹ Indian Institute Of Technology, Hyderabad

² Tata Institute of Fundamental Research, Hyderabad

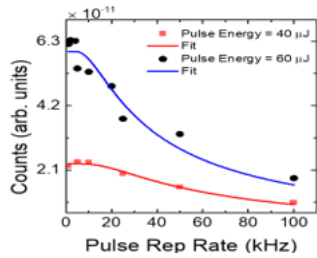
Electron emission from nanometer-scale metallic tips has gained significant interest due to field enhancement at the apex, enabling emission at lower intensities [1]. Laser-induced field emission from sharp tips has paved the way for ultrafast pulsed electron sources

with high spatiotemporal resolution. While previous studies focused on light polarization and incidence angle effects [2], we investigate the influence of laser pulse repetition rate on electron emission from a tungsten nanotip.

A tungsten nanotip (100 nm radius) was fabricated via electrochemical etching and characterized using SEM and an automated computer vision-based method [3]. A femtosecond laser (170 fs, 1.034 μm) with tunable repetition rate (1–100 kHz) was loosely focused onto the nanotip inside a 10^{-7} mbar vacuum chamber. The laser polarization was aligned parallel to the tip shaft, and a 600V DC bias was applied. Electron emission was detected using an MCP-phosphor screen assembly. Imaging a micron-scale copper mesh confirmed the nanometric origin of the emission. Our findings provide crucial insights into optimizing ultrafast electron sources, advancing applications in ultrafast imaging and coherent electron beam generation. The schematic of the experimental setup is given in Fig[(a)]. The repetition rate of laser was varied from 1KHz to 100KHz



by keeping the pulse energy constant, 40 μJ and 60 μJ . Repetition rate dependance of electron emission from nanotip is given in Fig[(b)].



The electron emission from the tip was found to decrease with increased repetition rate of the laser. This observation may be attributed to the microscopic local electron distribution on the tip. Considering the following model:

$$\frac{\partial n}{\partial t} = b(n_e - n) \quad (1)$$

This equation is similar to the diffusion equation, where the rate of change of electron density is proportional to the difference between the density at time t , $n(t)$ and the equilibrium density n_e

Integrating the above equation, we obtain:

$$n(t) = n_e \left(1 - k e^{-bt} \right) \quad (2)$$

where the parameter $\frac{1}{b}$ is the relaxation time.

Using the boundary condition at $t = 0$ just after electron tunneling:

$$k = \left(1 - \frac{n(0)}{n_e} \right) \quad (3)$$

which implies:

$$n_e k = (n_e - n(0)) \quad (4)$$

When the pulse energy is higher, the initial density $n(0)$ should be smaller. Consequently, $n_e k$ should be higher. This result is in agreement with our experimental findings.

To conclude, the laser repetition rate can be used as a parameter to control the electron emission from nanotip which can be used as an efficient source for time-resolved electron interferometry and for time-resolved nanometric imaging.

References

- [1] Hommelhoff, Peter and Kealhofer, Catherine and Kasevich, Mark A., "Ultrafast Electron Pulses from a Tungsten Tip Triggered by Low-Power Femtosecond Laser Pulses", *PhysRevLett.* 97.247402(2006)
- [2] Yanagisawa, Hirofumi and Hafner, Christian and Doná, Patrick and Klockner, Martin and Leuenberger, Dominik and Greber, Thomas and Osterwalder, Jurg and Hengsberger, Matthias, "Laser-induced field emission from a tungsten tip: Optical control of emission sites and the emission process", *PhysRevB.* 81.115429(2010).
- [3] Wei-Tse Chang, Ing-Shouh Hwang, Mu-Tung Chang, Chung-Yueh Lin, Wei-Hao Hsu, Jin-Long Hou, "Method of electrochemical etching of tungsten tips with controllable profiles", *Rev. Sci. Instrum.* 83 (8): 083704(2012)

#A61: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Strong electron-electron-nuclei correlations in multiphoton single and double ionization

Kilian Arteaga¹; Johannes Feist¹; Denis Jelovina¹; Fernando Martin²; Alicia Palacios Cañas³

¹ Universidad Autónoma de Madrid

² Universidad Autonoma de Madrid and IMDEA Nanoscience

³ Universidad Autonoma de Madrid

Attosecond spectroscopy have been mostly performed to date using table-top experimental set ups employing high-harmonic generation (HHG) techniques. The success of this technology was recognized with the Nobel Prize in Physics in 2023. Additionally, in the last decade, free electron laser (FEL) facilities have been commissioned all over the world, generating high brilliance and high intense pulses with incomparable frequency tunability, and, in some cases, even producing coherent attosecond pulses after the introduction of self-amplified spontaneous emission (SASE) schemes. The combination of these intense XUV sources with advanced detection devices that enable coincident measurements of all charged fragments enables a complete dynamical characterization of non-linear phenomena in the XUV and X-Ray regimes that remained experimentally inaccessible until now [1]. This technological progress thus calls for accurate and reliable theoretical methods to unravel the role of nuclear motion and electron correlation in the excitation and ionization process. We here present our first results obtained from a full dimensional solution for the two-photon double ionization of H₂ molecule. Very few theoretical works have addressed this problem due to difficulty and computational cost of achieving an accurate evaluation of the strong correlation between all fragments in the four-body Coulomb breakup, and only frozen-nuclei approaches have been employed until now [2]. In this work, we have implemented a new computational tool to describe, for the first time, the multiphoton double ionization of H₂ including electronic and nuclear degrees of freedom at equal footing, i.e., working beyond the Born-Oppenheimer approximation [4,5]. We employ a numerical representation of the molecular wave function directly written in a basis set of FE-DVR (finite elements combined with a discrete variable representation) and apply an exterior complex scaling procedure to impose the appropriate many-body Coulomb boundary conditions [3]. Accurate angle and energy differential two-photon double ionization yields show a significant energy displacements in the photoelectrons spectra with respect to frozen nuclei approaches. More interestingly, counter-intuitive angularly resolved double ionization yields with respect to its atomic analog are found, due to novel interferences that arise from sequential two-photon absorption paths through different cationic states

[5].

- [1] “Coulomb explosion imaging of small polyatomic molecules with ultrashort x-ray pulses”, X. Li et al., *Phys. Rev. Research* 4, 013029 (2022)
- [2] “Alignment and pulse-duration effects in two-photon double ionization of H₂ by femtosecond XUV laser pulses”, X. Guan et al., *Phys. Rev. A* 90, 043416 (2014)
- [3] “Practical calculations of quantum breakup cross sections”, C. W. McCurdy and T. N. Rescigno, *Phys. Rev.* 74, 052702 (2000) & “Double photoionization of aligned H₂”, *Phys. Rev. A* 74, 052702 (2006)
- [4] “A pump probe scheme with a single chirped pulse to image electron and nuclear dynamics in molecules”, D. Jelovina, J. Feist, F. Martín and A. Palacios, *New J. Phys.* 20, 123004 (2018)
- [5] “Strong Electron-Electron-Nuclei Correlations in Two-Photon Double Ionization of H₂”, K. Arteaga, J. Feist, D. Jelovina, F. Martín, A. Palacios, *Physical Review Letters* 133 (12), 123201 (2024)

#A62: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

The role of dephasing in solid-state high harmonic generation

Francisco Navarrete; Dieter Bauer

Institute of Physics-University of Rostock

Accurately reproducing the discrete spectral peaks observed in solid-state high-order harmonic generation (HHG) typically requires the explicit inclusion of dephasing effects [1, 2]. Here, we contrast numerical simulations with analytical modeling to clarify how dephasing affects both the spectral structure and the driver field dependence of the harmonics, with particular emphasis on the non-integer contributions in the plateau region. The HHG spectra are obtained both numerically, by performing a crystal-momentum resolved calculation of the time-dependent Schrödinger equation with multiple valence and conduction bands, and analytically, by implementing the semiconductor Bloch equations within a reduced two-band model treated by a saddle-point approximation [3]. From the latter, we derive closed-form expressions for the non-integer harmonics, which are in quantitative agreement with our simulations. The results shed light on the underlying electron dynamics, reveal the mechanisms that shape the HHG spectrum, and suggest concrete experimental strategies for resolving the persistent discrepancies between current theories and measurements.

- [1] Vampa et al. *Phys. Rev. Lett.* 113, 073901 (2014)
- [2] Cavaletto et al. *Nat. Rev. Phys.* 7, 38 (2025)
- [3] Navarrete et al., *Phys. Rev. A* 100, 033405 (2019)

#A63: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Modelling of photoionization time-delays in iodine-containing molecules with scalar relativistic effects

Jakub Benda; Martin Crhán; Zdeněk Mašín

Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, Prague 8, 180 00, Czechia

We present results of calculations of attosecond delays [1] in molecules containing heavy atoms and a methodology for inclusion of relativistic effects.

We focus on streaking delays in iodoalkanes at high photon energies around 100 eV, which probe the iodine 4d shell. In collaboration with the experimental group of R. Kienberger of TU Munich our ultimate aim is to understand streaking from such molecules deposited on surfaces. As a first step we focus on the study of an isolated iodine atom and the CH₃I molecule in the laboratory and molecular frames. Our goal is to accurately describe the effect of the iodine “giant dipole resonance” [2,3] on time-delays in both atomic and molecular environments.

To do this, we use the UKRmol+ suite [4] employing the R-matrix scheme, which is able to calculate a number of photoionization observables including the 1-photon Wigner and 2-photon RABITT delays. Within the suite our photoionization models are able to clearly separate collective effects from mean field ones. Our work also highlights that in the case of the polar CH₃I molecule in the molecular frame it is crucial to properly include the so-called “dipole-laser dressing” [6] in both the neutral and the ionized molecule.

We employ the newly implemented functionality of UKRmol+ to use “effective core potentials” [5] to include scalar relativistic effects originating in the inactive core electrons. To describe the scalar and spin-orbit relativistic effects for the active electrons we are utilizing the Breit-Pauli Hamiltonian in combination with the “Distorted Wave Born” approach of arbitrary order. We have successfully implemented this approach in the R-matrix scheme for model 1-electron problems and are working on the implementation in the multi-electron UKRmol+ suite.

- [1] Pazourek, R., et al. (2015). *Reviews of Modern Physics*, 87(3) 765-802.
- [2] Biswas, S., et al. (2020). *Nature Physics*, 16(7) 778-783.
- [3] Lindle, D. W., et al. (1984). *Physical Review A*, 30(1) 239.
- [4] Mašín, Z., et al. (2020). *Computer Physics Communications*, 249, 107092.
- [5] Reiher, M., & Wolf, A. (2015). John Wiley & Sons.
- [6] Benda, J., & Mašín, Z. (2024). *Physical Review A*, 109(1) 013106.
- [7] Scott, N. S., & Burke, P. G. (1980). *Journal of Physics B*, 13(21) 4299.

#A64: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Photo-modified birefringence of low thermal noise crystalline AlGaAs mirror coatings for ultrastable lasers

Chun Yu Ma; Jialiang Yu; Thomas Legero; Sofia Herbers; Daniele Nicolodi; Mona Kempkes; Fritz Riehle; Uwe Sterr

PTB Physikalisch-Technische Bundesanstalt

Ultrastable lasers locked to Fabry-Perot resonators are an important part of optical clocks, providing narrow bandwidth radiation for the excitation of clock transitions and acting as flywheel during deadtimes. The best systems operated at both room and cryogenic temperatures are limited by Brownian thermal noise of the dielectric mirror coatings [1-2]. Crystalline AlGaAs mirror coatings due to their low mechanical loss reduce this limit. However, the original birefringence of these coatings is unexpectedly modified by light which introduces technical photo-birefringent noise due to laser power fluctuation [3-4] as well as power driven spontaneous fluctuations of the birefringence (i.e. birefringent noise) [3,5]. After suppression of these noise contributions, the achieved frequency stability is still above the expected low thermal noise floor [3,5]. The source of this noise (global excess noise) is still yet to be further investigated.

We have further investigated the birefringent property of these coatings on a 48-cm long ULE cavity at room temperature, in particular on how light at different wavelengths influences the static birefringence of the crystalline coatings. Two independent lasers with wavelength of 1542 nm are locked to fast and slow polarization eigenmodes of

this cavity respectively as in previous investigations. A step in intracavity power modifies the static birefringence of the mirror coatings on timescales of a second, with faster response at higher final intracavity power [3,6]. We also investigate the modification of the coating birefringence from illumination by external LED light at different photon energies. Our results point to a two photon mechanism for photon energy below the bandgap of GaAs/AlGaAs or single photon mechanism at energies above the bandgap. By compensating the birefringent response with the polarization-independent thermal response on fast polarization mode, a fractional frequency instability of 4.8×10^{-17} (expressed in modified Allan deviation) could be demonstrated from a three-corned hat comparison with two other independent lasers locked to ultrastable cryogenic silicon cavities.

Our findings might help to understand the physical mechanisms of the photo-induced birefringent effect of these coatings, and thus enable improved designs of crystalline coatings, finally realizing their envisioned low Brownian thermal noise.

- [1] M. Schioppo et al., Nat. Commun., 13, 212 (2022)
- [2] D. G Matei et al., Phys. Rev. Lett., 118, 263202 (2017)
- [3] J. Yu et al., Phys. Rev. X, 13, 041002 (2023)
- [4] B. Kraus et al., Opt. Lett. 50, 658-661 (2025)
- [5] D. Kedar et al., Optica, 10, 464 (2023)
- [6] C. Y. Ma et al., J. Phys.: Conf. Ser. 2889, 012055 (2024)

#A65: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Multi-species cold-atom interferometry for inertial measurements

Alexandre Bresson¹; Alexis Bonnin¹; Antoine Godard²; Mal Landru¹; Malo Cadoret³; Nassim Zahzam¹; Sylvain Schwartz¹; Yannick Bidet¹

¹ ONERA DPHY-SLM

² ONERA DSG

³ LCM-CNAM

Using wave properties of matter, cold atoms can become tiny quantum sensors with high stability and sensitivity to inertial quantities, such as rotation or acceleration. The principle of a cold-atom gravimeter is the following: cold atoms (a few μK) free fall in an ultra-high vacuum chamber, submitted to the Earth gravity g . While they are falling, one can probe the atoms with lasers in a matter-wave Mach-Zehnder interferometer: carefully-tuned laser pulses will transfer momentum to the atoms which will result in the matter wave being separated, deflected and recombined. At the end of the interferometer one can get the value of g by measuring the phase of the atoms via fluorescence. Contrary to their classical counterparts, cold-atom accelerometers suffer from dead times between each measurement (corresponding to the laser cooling sequence) and have a limited measurement range. However, they do benefit from an unrivalled stability and allow to perform absolute measurements [1]. Since classical and atomic sensors have complementary strengths and weaknesses, they are both commonly combined to create hybrid sensors. Unfortunately, hybrid sensors could be limited by the intrinsic noise of the classical sensor. However, there could be another way to make the best of the atomic accelerometer: manipulating different atomic species simultaneously inside the same sensor. Indeed, there are insightful configurations using 3 atomic species (^{85}Rb , ^{87}Rb and ^{133}Cs) instead of one. One could decrease dead times by "juggling" between the 3 species such that while one species is being laser-cooled, the other is free-falling in the matter-wave Mach-Zehnder and the third species is being detected. Another configuration could enable simultaneous 3D acceleration measurements. The challenge is to imagine and set up ingenious configurations to exploit the full potential of the triple species gravimeter, dealing with inter-species interactions while keeping the set-up compact and robust for possible applications in dynamic environment. In this regard, we have developed an all-fibered laser system based on telecom laser diodes at

1.5 μm and at 1.9 μm .

A first triple species magneto-optical trap has been obtained and its characteristics such as the loading time or the number of atoms are to be studied, as they contain information on the collision processes. Meanwhile, a numerical simulation is developed to investigate the impact of deadtimes in the context of on-board measurements, as well as highlight the benefits of a triple-species continuous measurement.

- [1] Bidet, Y. et al., Absolute marine gravimetry with matter-wave interferometry. Nature Commun, <https://doi.org/10.1038/s41467-018-03040-2>

#A66: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Coupled atom-cavity systems for quantum-enhanced metrology: adiabatic elimination of the cavity mode beyond the leading order

Gianluca Bertaina¹; Giulia Dellea²; Marco G. Genoni²; Marco G. Tarallo¹; Stefano Gregorio Giaccari¹

¹ Istituto Nazionale di Ricerca Metrologica (INRiM)

² Università degli Studi di Milano

Spin-squeezed states are a prototypical example of metrologically useful states where structured entanglement allows for enhanced sensing with respect to the one possible using classically correlated particles. Relevant aspects are both the efficient preparation of spin-squeezed states and the scalability of estimation precision with the number N of probes. Recently, in the context of the generation of spin-squeezed states via coupling of three-level atoms to an optical cavity and continuous quantum measurement of the transmitted cavity field, it was shown that increasing the atom-cavity coupling can be detrimental to spin-squeezing generation, an effect that is not appreciated in the standard second-order cavity removal approximation [1]. We describe adiabatic elimination techniques to derive an effective Lindblad master equation up to third order in the collective spin operators. We then discuss two approaches to the solution of this equation: a very general one based on a systematic implementation of the truncated cumulant expansion and its numerical solution, which allows to show that the mean field and Gaussian approximations are inadequate to predict the correct spin-squeezing scaling, and a fully analytic one leveraging on the existence of a complete set of commuting weak symmetries [2].

References

- [1] A. Capritti, M. Barbiero, M. G. Tarallo, M. G. Genoni and G. Bertaina, Quantum Sci. Technol., 9, no.3, (2024) 035032
- [2] S. G. Giaccari, G. Dellea, M. G. Genoni and G. Bertaina, in preparation

#A67: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Towards the Assembly of YbCaF

Benjamin Fox; Luke Caldwell; Samuel Haswell

university college London

This research project investigates the development and use of the tri-

atomic molecule YbCaF for measuring the magnetic quadrupole moment (MQM) of the Yb-173 nucleus. This property is of interest as it breaks CP symmetry, contributing to the understanding of matter-antimatter asymmetry. The YbCaF molecule is ideal for this: the quadrupole-deformed Yb-173 nucleus enhances the size of the MQM for a given new physics scenario, and the molecule's bent structure facilitates parity doublets, a powerful tool for uncovering and rejecting systematic errors. We aim to laser cool both Yb and CaF, then trap them in optical tweezers and combine them into molecules. Our current progress focuses mainly on the preparation of Yb, with the apparatus being constructed to cool the atoms to a point where they can be trapped.

#A68: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Temperature Dependence of ac Stark Shift in a Vapor Cell Rb Atomic Clock

Hyun-Gue Hong; Jae Hoon Lee; Jaek Baek; Meung Ho Seo; Sang Eon Park; Sang-Bum Lee; Sangwon Seo; Seji Kang; Soyeon Choi; Taeg Yong Kwon; Young-Ho Park

KRISS (Korea Research Institute of Standards and Science)

Light shift, or ac Stark shift, plays an important role in vapor cell frequency standards, and substantial efforts have focused on minimizing its impact on frequency stability. Its temperature dependence is, on the other hand, generally considered negligible compared to the pressure shift arising from buffer gas collisions. Thus, it is of primary concern to find the so called inversion temperature at which the first-order sensitivity vanishes by proper choice of buffer gas species. However, in laser-pumped alkali vapor cells, spatial inhomogeneity of laser intensity along the propagation axis can introduce a notable temperature dependence, and the combined effect of collisional and light shifts in coherent population trapping resonances has been observed.

In this work, we present a comprehensive study on how the inversion temperature in a double-resonance Rb clock can be tuned by varying the laser intensity. Our findings reveal that even with a commonly used optical path length of 25 mm, laser attenuation within the cell can induce a significant, non-trivial temperature dependence of the light shift. For a set of the pressures of argon and nitrogen, we observed a transition from a collision-shift-dominated regime to a light-shift-dominated regime as the laser intensity increased, clearly demonstrating the characteristic temperature dependence of the light shift. We developed a simple theoretical model incorporating optical density and absorption line shifts, which was validated by independent measurements of the light shift versus laser frequency. These results offer practical insights for improving the robustness of laser-pumped miniature atomic clocks.

#A69: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Status of Rb Two-Photon Optical Clock with a Chip-Scale Vapor Cell at KRISS

Kyung Bin Park¹; Jae Hoon Lee²; Hyun-Gue Hong²; Myoungcho Seo²; Jongchul Park³; Yeeun Na³; Hansuek Lee⁴; Dai Hyuk Yu²

¹ Korea Research Institute of Standards and Science, Korea Advanced Institute of Science and Technology

² Korea Research Institute of Standards and Science

³ National NanoFab Center

⁴ Korea Advanced Institute of Science and Technology

We develop a compact optical frequency reference system based on the two-photon transition between the $5S_{1/2}$, $F=2$ state and $5S_{5/2}$, $F=4$ states of ^{87}Rb atoms in a microfabricated chip-cell, which was successfully implemented for frequency stabilization of a self-referenced SBS microcomb [1]. A 1556 nm laser (DFB1550p, Thorlabs) was used in conjunction with a second-harmonic generation (SHG) module (WH-0778-000-F-B-C, NTT) to generate the 778.1 nm two-photon excitation beam, and a fiber-based optical path was designed to ensure robust beam alignment during portable operation. The system integrates a magnetic-shielded housing that contains the Rb chip-cell, dichroic filters, a micro photomultiplier tube (H12405, Hamamatsu), and optical lenses. We also utilize counter-propagating beams to achieve Doppler-free two-photon absorption spectroscopy, resolving the hyperfine structure of ^{87}Rb . The observed transition exhibited a full width at half maximum (FWHM) of 1.52 MHz based on Lorentzian fitting. Frequency modulation was applied using a fiber-coupled AOM, enabling extraction of an error signal from the two-photon transition, which was effectively used for laser frequency locking and system characterization.

[1] I. H. Do, D. Kim, D. Jeong, D. Suk, D. Kwon, J. Kim, J. H. Lee, and H. Lee, "Self-stabilized soliton generation in a microresonator through mode-pulled Brillouin lasing," *Opt. Lett.* **46**, 1772 (2021)

#A70: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Floquet Theory of Sequential Bragg and Bloch Oscillation Based Large Momentum Transfer

Patrik Mönkeberg¹; Ashkan Alibabaei¹; Florian Fitzek¹; Naceur Gaaloul¹; Klemens Hammerer²

¹ Leibniz Universität Hannover

² Leibniz University Hannover

Large momentum transfer techniques are essential tools to enhance the sensitivity of atom interferometers. So far, elastic scattering processes like Bloch Oscillations and sequential Bragg diffraction have proven to be effective means of implementing large momentum transfer. To fully exploit the potential of these methods, an accurate theoretical description is crucial. In this work, we utilize a Floquet theoretical approach to describe both Bloch Oscillations and sequential Bragg diffraction as two limiting cases of a more general framework. We verify its accuracy through comparison with an exact numerical solution of the Schrödinger equation. Using our approach, we investigate the efficiency and limits of the covered large momentum transfer pulses. We compare these results to current state-of-the-art experiments.

#A71: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Direct comparison of polarizability measurements with a dual-species ion clock

Ekkehard Peik¹; Jian Jiang¹; Marianna Safronova²; Martin Steinel¹; Melina Filzinger¹; Nils Huntemann¹; Saaswath JK¹; Thomas Lindvall³

¹ Physikalisch-Technische Bundesanstalt

² University of Delaware

³ National Metrology Institute VTT MIKES

Atomic clocks realize unperturbed transition frequencies of atoms or ions. For clocks operated at room temperature, the Stark shift from thermal radiation of the environment causes the largest frequency shift and needs to be corrected for with high accuracy. In ion-based systems two methods have been employed to assess the sensitivity of the transition frequency to room-temperature blackbody radiation. For most ion species, the differential polarizability $\Delta\alpha$ is obtained via frequency shifts from intense laser radiation at infrared or near-infrared wavelengths. The intensity of the perturbing laser field is derived from estimations of the intensity profile at the position of the trapped ion and the optical power of the beam. Here, uncertainties of a few percent result from the optical power measurements and the limited knowledge of the intensity distribution [1, 2].

More accurate determinations are possible, if the Stark shift increases the reference transition frequency, which corresponds to a negative differential polarizability. In this case, the sensitivity can be calculated from the “magic” frequency of the field trapping the ion. Here, the Stark and relativistic Doppler shift from excess micromotion, the driven motion of the ion in the trapping field, cancel. For Sr^+ and Ca^+ clock transitions $\Delta\alpha$ has been measured with uncertainties of 0.15% and 0.06% [3, 4].

We present results from a complementary measurement of $\Delta\alpha$ for the $^{88}\text{Sr}^+$ clock transition using perturbing laser radiation. Interestingly, we find a difference of 13% corresponding to 4σ significance between the two approaches. By operating a dual species clock with $^{171}\text{Yb}^+$ and $^{88}\text{Sr}^+$, we can subject both ion species to the same laser intensity and measure their polarizability ratio. We find that the ratio is consistent with independent determinations of the polarizability for each ion species using perturbing laser radiation. But they show the same discrepancy to the polarizability obtained via the “magic” trap drive frequency, supporting that the disagreement is due to the methods themselves. We aim to determine which value of the Sr^+ polarizability is correct with a direct measurement of the $^{88}\text{Sr}^+$ frequency at different environmental temperatures.

[1] N. Huntemann et al., “Single-Ion Atomic Clock with 3×10^{-18} Systematic Uncertainty”, *Phys. Rev. Lett.* 116, 063001 (2016)

[2] K. J. Arnold et al., “Blackbody radiation shift assessment for a lutetium ion clock”, *Nature Communications* 9, 1650 (2018)

[3] P. Dubé et al., “High-Accuracy Measurement of the Differential Scalar Polarizability of a $^{88}\text{Sr}^+$ Clock Using the Time-Dilation Effect”, *Phys. Rev. Lett.* 112, 173002 (2014)

[4] Y. Huang et al., “ $^{40}\text{Ca}^+$ ion optical clock with micromotion-induced shifts below 1×10^{-18} ”, *Phys. Rev. A* 99, 011401(R) (2019)

#A72: Quantum technologies, quantum optics, cavity QED, quantum information

Collective Quantum Phenomena

Raphael Holzinger

University of Innsbruck / Harvard University

Recent advancements in quantum optics have significantly enhanced our understanding of interactions between quantum emitters, driving progress in quantum technologies. Collective phenomena emerge when multiple quantum emitters interact via a shared electromagnetic mode, leading to effects like correlated decay and coherent photon exchange and the coupling of two-level quantum emitters to a common electromagnetic reservoir presents a promising platform for exploring superradiance, subradiance, and nonlinear quantum effects.

#A73: Quantum technologies, quantum optics, cavity QED, quantum information

Rapid and Robust Hyperfine Qudit Gates in Trapped Neutral Atoms

Johannes K. Krondorfer; Matthias Diez; Andreas W. Hauser

Graz University of Technology, Institute of Experimental Physics

Neutral atoms trapped in optical potentials have emerged as a rapidly progressing platform for quantum information processing. Alkaline-earth and alkaline-earth-like atoms are particularly attractive due to their long-lived qubit states, the theoretically well-understood hyperfine structure, and the ability to precisely control their interactions with external fields. Among these systems, ^{87}Sr stands out for its exceptional coherence times, making it a leading candidate for qubit encoding and quantum information storage. Beyond qubits, the rich level structure of ^{87}Sr enables the use of multi-level qudits, which offer additional computational advantages, including increased information density and reduced circuit complexity.

We propose fast and robust single qudit gates in ^{87}Sr using optical nuclear electric resonance (ONER). ONER exploits the nuclear hyperfine interaction in an appropriate excited state, via suitably detuned, polarized and amplitude-modulated laser light, to drive nuclear spin transitions of the hyperfine ground states. By investigating the hyperfine structure of the $5s^2\ ^1S_0 \rightarrow 5s5p\ ^3P_1$ optical transition in neutral ^{87}Sr , we identify the magnetic field strengths and laser parameters necessary to drive multiple spin transitions. Our simulations show that ONER could enable faster spin operations compared to the state-of-the-art oscillations in this ‘atomic qudit’. Moreover, we show that the threshold for fault-tolerant quantum computing can be surpassed even in the presence of typical noise sources.

These results pave the way for significant advances in nuclear spin control, opening new possibilities for quantum memories and other quantum technologies.

#A74: Quantum technologies, quantum optics, cavity QED, quantum information

Hot Schrödinger Cat States

Ian Yang¹; Thomas Agrenius²; Vasilisa Usova¹; Oriol Romero-Isart³; Gerhard Kirchmair¹

¹ University of Innsbruck, Institute for Experimental Physics

² University of Innsbruck, Institute for Theoretical Physics

³ ICFO - Institut de Ciències Fotoniques

The observation of quantum phenomena often necessitates sufficiently pure states, a requirement that can be challenging to achieve. In this study, our goal is to prepare a non-classical state originating from a mixed state, utilizing dynamics that preserve the initial low purity of the state. We generate a quantum superposition of displaced thermal states within a microwave cavity using only unitary interactions with a transmon qubit. We measure the Wigner functions of these “hot” Schrödinger cat states for an initial purity as low as 0.06. This corresponds to a cavity mode temperature of up to 1.8 Kelvin, sixty times hotter than the cavity’s physical environment. Our realization of highly mixed quantum superposition states could be implemented with other continuous-variable systems e.g. nanomechanical oscillators, for which ground-state cooling remains challenging.

#A75: Quantum technologies, quantum optics, cavity QED, quantum information

Unconventional Phonon blockade effect in a coupled nanomechanical system quadratically coupled to a two-level system

Bhaskar Kumar¹; Soumya Kanti Das²; Chandan Samanta²; Prabhu Rajagopal¹

¹ Indian Institute of Technology, Madras

² Indian Institute of Science Education and Research, Bhopal

Phonon antibunching or phonon blockade effect (PBE), a hallmark of quantum mechanical behavior in vibrational systems, offers promising prospects in quantum information processing and phonon-based quantum computing. In this work, we explore the phenomenon of phonon antibunching in a system comprising two coupled nanomechanical resonators (NAMRs) interacting with a two-level system (TLS). We derive the system’s Hamiltonian and analyze the antibunching behavior by numerically simulating the second-order correlation function using the Lindblad master equation. By examining the second-order correlation function, we demonstrate phonon antibunching that arises from quantum interference between distinct excitation pathways. The key features highlighting our work is due to the presence of two different coupling mechanisms. The first NAMR is linearly coupled to the second NAMR, which has a weak Duffing nonlinearity, while the second NAMR is quadratically coupled to the TLS. The system leverages the interplay between the two different coupling mechanisms to achieve a strong antibunching effect even in a weak coupling regime. The optimal antibunching conditions are achieved by tuning the coupling strength and detuning parameters between the resonators and the TLS. Moreover, by tuning the phase difference and amplitude of two external driving fields, destructive interference between the two-phonon excitation can be maximized, enhancing the PBE. We also show the temperature resilience of the design by analyzing its robustness against thermal noise induced by temperature variations. This study provides a framework for achieving strong phonon antibunching in coupled resonator-TLS systems, paving the way for the experimental realization of single-phonon sources and advancing quantum acoustics applications.

#A76: Quantum technologies, quantum optics, cavity QED, quantum information

Full-stack neutral-atom quantum computing with 85Rb

Yuri van der Werf; Deon Janse van Rensburg; Edgar Vredendregt; Jesús del Pozo Mellado; Rianne Lous; Rogier Venderbosch; Servaas Kokkelmans

Eindhoven University of Technology

The Neutral Atom KAT-1 Collaboration is working on the realisation of a full-stack quantum computing solution, with a quantum processing unit (QPU) based on neutral atoms with Rydberg interactions, trapped in optical tweezer arrays. Out of a total of three QPU setups: a first generation ⁸⁸Sr system in Amsterdam and the 2nd generation ⁸⁸Sr setup in Eindhoven, this work concerns the ⁸⁵Rb demonstrator system at Eindhoven University. The relatively low complexity of Rb laser cooling combined with a robust Artiq control system, as well as intermittent scheduling of calibration routines and machine-learning based optimization runs, ensure that the setup can be operated remotely and is operational 24 hours per day.

The ⁸⁵Rb qubit is based on the $|F=2, m_F=0\rangle \rightarrow |F=3, m_F=0\rangle$ clock transition, which is driven with 3 GHz microwaves, offering a robust single-qubit gate drive. Our coherence times are in the tens to hundreds of milliseconds range which, combined with a 0.1 MHz Rabi frequency, allows for long qubit control sequences. For the qubit driving we use a Quantum Machines Operator-X module, which enables us to implement complex pulse shapes on a fast timescale with excellent phase control, for robust pulses and optimal control applications. As a first demonstration we have implemented proof-of-principle experiments on theoretical qubit-drive noise models, which show excellent agreement with analytical results and simulations.

The qubit control toolbox will be completed with the addition of a Stark-shifting laser for single qubit addressing through local Z rotations and two-photon Rydberg excitation to the 60S level, which are both currently under development. The ⁸⁵Rb demonstrator system forms an ideal platform for collaboration with our theory department, which focuses on the development of neutral-atom-specific quantum algorithms and optimal control techniques. This serves as the first step in enabling third-party access to our QPUs via the Quantum Inspire platform.

#A77: Quantum technologies, quantum optics, cavity QED, quantum information

Reconstruction of Quantum Gates using Quantum Process Tomography

Arash Dezhang Fard¹; Adam Miranowicz²; Marek Kopciuch²; Szymon Pustelny³; Yujie Sun¹

¹ Jagiellonian University

² Adam Mickiewicz University

³ Harvard University

Reconstruction of Quantum Gates using Quantum Process Tomography

Arash Dezhang Fard^{1,2}, Yujie Sun¹, Marek Kopciuch⁴, Adam Miranowicz⁴, Szymon Pustelny^{1,3}

¹ Marian Smoluchowski Institute of Physics, Jagiellonian University in Krakow, 30-348 Krakow, Poland

²Doctoral School of Exact and Natural Sciences, Jagiellonian University in Krakow, 30-348 Krakow, Poland

³Department of Physics, Harvard University, Cambridge, MA 02138, USA

⁴Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University, 61-614 Poznan, Poland

Quantum gate reconstruction plays a crucial role in quantum computing by enabling the verification and characterization of quantum operations. Quantum Process Tomography (QPT) is a powerful technique that is used to fully reconstruct the process matrix of a quantum gate, providing a comprehensive understanding of its behavior. By utilizing QPT, one can identify imperfections in quantum gates, making it an essential tool for the development of reliable quantum computing systems.

In this study, we present our experimental investigations on the reconstruction of quantum gates using the QPT technique in the qutrit system. The core of our experimental setup is a room-temperature ^{87}Rb atomic vapor cell, which contains two hyperfine ground states with $F = 1$ and $F = 2$ (F is the total angular momentum). To achieve a qutrit system, the $F = 2$ state is depleted using a laser beam. To perform the QPT, a set of initial states corresponding to the Gell-Mann matrices is chosen. By comparing initial states with their evolved counterparts, we gain insight into the quantum process. For more insightful characterization of the measured process, we reconstructed the minimal set of Kraus maps that describe measured process. We demonstrate the reconstruction of some fundamental quantum gates, showcasing the high precision of the gate reconstruction using the QPT technique [1,2,3].

1. A. D. Fard, M. Kopciuch, and Y. Sun, P. Włodarczyk, and S. Pustelny, Isolating Pure Quadratic Zeeman Splitting, arXiv, 2412.07610, 2024.
2. Y. Sun, M. Kopciuch, A. D. Fard, A. Miranowicz, and S. Pustelny Quantum Process Tomography of Room-Temperature Alkali-Metal Vapor, In preparation.
3. A. D. Fard, Y. Sun, M. Kopciuch, A. Miranowicz, and S. Pustelny Reconstruction of Quantum Gates via Quantum Process Tomography, In preparation.

#A78: Quantum technologies, quantum optics, cavity QED, quantum information

Utilizing the center of mass for sensing magnetic fields and gravity in a cold atom cavity QED system with magnetic trapping

Alexandra Simon; András Dombi; Árpád Kurkó; Dániel Varga; Dávid Nagy; Péter Domokos; Thomas William Clark; András Vukics

HUN-REN Wigner Research Centre for Physics

We investigate a cold ensemble of magnetically trapped ^{87}Rb atoms, that can be magnetically transported into a high-finesse optical cavity. Within the cavity, the atoms are either kept in the magnetic trap, or transferred into a cavity-sustained optical dipole trap [1]. The cloud can be diagnosed by the scattering of a transverse laser into the cavity, where the resulting cavity field is monitored through one of the mirrors by single-photon detection after separating vertically and horizontally polarized photons.

With this system, we first exhibit the ‘cold atom buoy’ technique. In the magnetic trap we take absorption images of the ensemble, and compare the center-of-mass positions under reversed magnetic quadrupole polarities that reverses the translation caused by external fields. This allows for determining the true geometrical center of the quadrupole, and sensing external homogeneous bias fields at the position of the atoms in an intermediary regime above the range of optically pumped magnetometry.

Further, after transporting the atoms into the cavity, and by analysing the polarization-resolved cavity output, we can distinguish between Rayleigh and Raman scattering from the atoms. Since the latter scattering type corresponds to redistribution on magnetic sublevels, it is sensitive to magnetic fields. As the magnetic trap is pulled through the cavity axis, this allows for using the cavity as a tomograph to separately map out the density distribution of the atomic cloud (Rayleigh scattering) versus the trapping magnetic field (Raman scattering), the two differing due to gravity. Hence the gravitational sag of a magnetically trapped cold ensemble can be characterized.

The experiment is controlled using the Wigner Time Python package [3], a data-oriented tool for defining timelines of real-time control for cold-atom experiments, that defines and manipulates experimental timelines as pandas DataFrames with a functional-type API. This approach enables transparent and flexible software control, with seamless integration with the broader scientific Python ecosystem.

[1] Varga, Dániel, et al. “Loading atoms from a large magnetic trap to a small intra-cavity optical lattice.” *Physics Letters A* 505 (2024): 129444.

[2] Gábor, Bence, et al. “Demonstration of strong coupling of a subradiant atom array to a cavity vacuum.” arXiv preprint arXiv:2408.17079 (2024).

[3] https://github.com/WignerQuantumOptics/Wigner_Time

#A79: Quantum technologies, quantum optics, cavity QED, quantum information

Quantum Annealing for Combinatorial Optimization and Many-Body Physics: Room Scheduling and $\mathbb{Z}_2$ Spin Liquid

Krzysztof Giergiel

CSIRO

We investigate the application of quantum annealing on the D-Wave Advantage 2 platform for both combinatorial optimization and quantum many-body physics. First, we explore room scheduling optimization for sports camps at the Australian Institute of Sport, formulating the problem as a binary integer programming task. By comparing classical, hybrid, and quantum annealing approaches, we assess embedding challenges and the feasibility of quantum solutions given current hardware limitations. We explore and propose solutions for problem-aware calibration, correcting long-range interactions detrimental to the model. Second, we investigate the experimental realization of a classical $\mathbb{Z}_2$ spin liquid using a native embedding on the Advantage 2 hardware. We present progress toward studying defect transport by initializing defects and tracking their evolution, demonstrating the potential of quantum annealing for probing emergent phenomena, even in noisy environments.

#A80: Quantum technologies, quantum optics, cavity QED, quantum information

Environment-Enhanced Single-Photon Absorption in a Nanoring of Dipole-Coupled Quantum Emitters

Eric Sánchez-Llorente¹; Arpita Pal²; Helmut Ritsch²; Maria Moreno-Cardoner¹

¹ Institut de Ciències del Cosmos, Universitat de Barcelona

² Institut für Theoretische Physik, Universität Innsbruck

Decoherence is usually considered detrimental in quantum information and quantum optics applications. However, the interplay between environment dynamics and unitary evolution can give rise to interesting quantum many-body phenomena and can even be harnessed to become a useful resource.

As it is well known, in dense atomic arrays coupled to a common radiation mode, collective spontaneous emission occurs, leading to the emergence of very subradiant states [1]. Here, we demonstrate how these modes in combination with additional decoherence mechanisms such as dephasing or a global thermalizing bath, can significantly enhance the single-photon absorption cross-section in nanorings of quantum emitters. The nanoring geometry is particularly appealing due to its unique optical properties [2] and its resemblance to natural light-harvesting complexes, which serve as efficient antennas in photosynthesis [3,4]. Despite the complexity of these biological systems, our findings suggest they may exploit similar principles, potentially shedding light on fundamental aspects of energy absorption and transfer in nature.

[1] A. Asenjo-Garcia, M. Moreno-Cardoner et al., PRX 7, 031024 (2017).

[2] M. Moreno-Cardoner, D. Plankensteiner, L. Ostermann, D.E. Chang, H. Ritsch, PRA 100, 023806 (2019).

[3] J.L. Herek et al., Nature 417, 533 (2002).

[4] M. Moreno-Cardoner, R. Holzinger, H. Ritsch, Optics Express 30, 10779 (2022).

#A81: Quantum technologies, quantum optics, cavity QED, quantum information

Protecting collective qubits

Antoine Covolo; Valentin Magro; Mathieu Girard; Sebastien Garcia; Alexei Ourjoumtsev

JEIP, UAR 3573 CNRS, Collège de France, PSL University

Collective atomic or solid-state excitations present important advantages for encoding qubits, such as strong directional coupling to light. Unfortunately, they are plagued by inhomogeneities between the emitters, which make the qubit decay into a quasi-continuum of dark states. In most cases, this process is non-Markovian. Through a simple and resource-efficient formalism, we unveil a regime where the decay is suppressed by a combination of driving and non-Markovianity. We experimentally demonstrate this “driving protection” using a Rydberg superatom, extending its coherent dynamics beyond the characteristic free decay time by an order of magnitude [1].

[1] A. Covolo et al, arXiv:2501.07232.

#A82: Quantum technologies, quantum optics, cavity QED, quantum information

Quantum Correlations in UV Dual-Comb Spectroscopy

Andrey Muraviev¹; Dimitrii Konnov¹; Konstantin Vodopyanov¹; Radmir Kokoulin²

¹ Center for Research and Education in Optics and Lasers, University of Central Florida, Orlando, Florida, USA

² University of Central Florida

We investigate intrinsic quantum correlations—such as polarization and quadrature entanglement—in the ultraviolet dual-comb output generated from a Cr:ZnS-based system operating at 2.4 μm . Using nonlinear crystals such as periodically poled lithium niobate (PPLN), we have coherently interfered harmonics up to the 7th order (330–390 nm) with sub-femtosecond timing precision and observed stable mode-resolved spectra exceeding 10^6 lines and resolving power ($\lambda/\Delta\lambda$) above 10^7 . In this study, we evaluate quadrature entanglement and quantum Fisher information from our archived dual-comb interferograms, assess the presence of quantum correlations, and explore implications for UV metrology and the future development of a nuclear clock.

Poster Session B

#B1: Atomic and molecular spectroscopy, photo-induced processes

Quantum Monte Carlo study on positron binding to atomic anion dimers

Masanori Tachikawa Tachikawa

Yokohama City University

Recently, it was found that the positronic complex with $(\text{H}^-)_2$ can form the stable bound state concerning the dissociation into $\text{H}^- + \text{PsH}$ by a positron mediate bonding. This bonding situation, which resembles the well-defined single covalent bond, was qualified as "positronic covalent bonding". On the other hand, a similar binding mechanism may be possible for anion dimers of other alkali species, such as lithium. In this study, we have investigated the stabilities of $[\text{X}^-; \text{e}^+; \text{X}^-]$ homonuclear systems with $\text{X} = \text{H}$ and Li using the quantum Monte Carlo method combined with the multi-component molecular orbital calculation.

Our results show that the system has a single energy minimum in all the PECs, and its internuclear distance is drastically shortened by improving the accuracy of interparticle correlation effects. According to the characteristics of the electron and positron densities, the energy minimum structure at the HF level appears like a positronic covalent bonding, whereas the compact structure predicted at the DMC level may have strongly delocalized characters of both one excess electron and a positron.

By evaluating PECs of both lower energy decays into $\text{Ps} + \text{Li}_2^-$ and $\text{Ps}^- + \text{Li}_2$, we confirmed that the $[\text{Li}^-; \text{e}^+; \text{Li}^-]$ system is stable for both these thresholds. The analytical results suggest that the dominant structure is depicted as Ps binding to Li_2^- anion, which is different from the $[\text{H}^-; \text{e}^+; \text{H}^-]$ case with a locally stable covalent positronic bonded structure.

#B2: Atomic and molecular spectroscopy, photo-induced processes

Cyclic C_4^+ as the carrier of diffuse interstellar band at 503.9 nm

Serge Krasnokutski¹; Lisa Ganner²; Milan Ončák²; Florian Foitzik²; Stefan Bergmeister²; Fabio Zappa²; Paul Scheier²; Elisabeth Gruber²

¹ Friedrich-Schiller-Universität Jena

² Universität Innsbruck

The diffuse interstellar bands (DIBs) have remained a mystery in astronomy since their discovery over a century ago. The only currently known carrier is C_{60}^+ responsible for five DIBs, while more than 550 are yet to be interpreted. The spectra of short carbon chain cations C_n^+ , which are considered one of the most promising classes of species for the role of carriers of DIBs, are successfully recorded using He-tagging spectroscopy. The comparison of laboratory spectra with the observations demonstrates a close match of two absorption bands of C_4^+ with the broad DIB at 503.9 nm. This defines a high abundance of these ions in the interstellar medium (ISM), which should exceed those of other similar-sized carbon chain cations. It is anticipated that all other short carbon chain cations will exhibit linear geometry and, as a consequence, will have a long vibrational progression. However,

the distinctive cyclic geometry of C_4^+ is postulated to underpin the elevated abundance of these ions in the ISM, as well as the distinctive spectrum of this ion, which displays a single strong, relatively narrow absorption band that exceeds in intensity all other absorption bands in the visible range.

#B3: Atomic and molecular spectroscopy, photo-induced processes

Characterization of the spectral signal of the double-well broad potential curve of NaH D state

Chin-Chun Tsai; Hsien-Yu Huang; Thou-Jen Whang

National Cheng-Kung University, Taiwan

Using pulsed optical-optical double resonance fluorescence depletion spectroscopy, many ro-vibrations of the $\text{NaH D}^1\Sigma$ state have been observed. The ab initio calculations show that the adiabatic potential energy curve of the $\text{NaH D}^1\Sigma$ state has a very shallow double-well structure, with completely different well widths giving different rotational constants and vibration spacing, while the high-energy region is another very wide potential well confined by an outer turning points of ionic interaction (characterized by the $1/R$ leading term). In this potential well, the rotation constant and vibration spacing have significantly different characteristics in different energy ranges, from which we can deduce the interaction force between NaH diatomic molecules. Due to predissociation, the linewidths of some rotational vibration energy levels are more than ten times wider than those of conventional depletion signals. In this presentation, we construct a hybrid potential curve modified from a theoretical curve to better represent the observed ro-vibration energy levels.

#B4: Atomic and molecular spectroscopy, photo-induced processes

Electron-Photon Coincidence Measurements at the Synchrotron Facility MAX IV during TRIBs operation mode

Adrian Krone¹; Andreas Hans¹; Andreas Hans¹; Antti Kivimäki²; Arno Ehresmann¹; Johannes Viehmann¹; Noelle Walsh²; Yusaku Terao¹

¹ Universität Kassel

² MAX IV Laboratory

Coincidence measurements are an important experimental tool in atomic or molecular physics. Our group has used electron-photon coincidence measurements to investigate rare gas clusters after synchrotron irradiation. More specifically, electron times-of flight and photon counts (UV-VUV) are recorded between two consecutive synchrotron pulses. However, to employ these coincidence measurements using electron time-of-flight detection techniques at synchrotron facilities requires so-called single bunch operation mode. This mode offers the needed time spacing in between synchrotron excitation pulses. Nevertheless, the lower synchrotron intensities makes this mode unattractive for many

users not reliant on this kind of time resolution.

Transverse Resonance Island Buckets (TRIBs) is an operation mode where a pseudo-single bunch in addition to 'conventional' multi bunch is accessible for users by aligning beamline optics to the respective orbitals of the bunches. Here, we present the first results from coincidence measurements during TRIBs operation mode at MAX IV.

#B5: Atomic and molecular spectroscopy, photo-induced processes

Mid-infrared frequency comb spectroscopy in uniform supersonic flows: A look into vibrational excitation in Laval nozzles

Lok Yiu (Kathy) Wu; Daniel I. Lucas; Madeleine E. Robertson; Julia H. Lehman

University of Birmingham

Over the past forty years, the CRESU (Cinétique de Réaction en Écoulement Supersonique Uniforme) technique has been a workhorse for investigating ion-molecule and neutral-neutral reactions in the low temperature regime [1], with temperatures reaching as low as 5.8 K [2]. The uniform supersonic flow, produced by a Laval nozzle, is known to be a wall-less, high-density flow of gas thermalised across all degrees of freedom [1, 3]. Recently, our group has combined a low temperature uniform supersonic flow with direct frequency comb spectroscopy (DFCS) for the first time [4], allowing the rotational and vibrational degrees of freedom of gases in the flow to be probed simultaneously. I will be presenting an overview of our new instrument, along with some of our first spectroscopic results.

[1] Rowe, B. R.; Canosa, A.; Heard, D. E. WORLD SCIENTIFIC (EUROPE) June 2022.

[2] Berteloite, C.; Lara, M.; Bergeat, A.; Le Picard, S. D.; Dayou, F.; Hickson, K. M.; Canosa, A.; Naulin, C.; Launay, J.-M.; Sims, I. R.; Costes, M. Phys. Rev. Lett. 2010, 105 (20).

[3] Sims, I. R.; Smith, I. W. M. Annu. Rev. Phys. Chem. 1995, 46 (1), 109–138.

[4] Lucas, D. I.; Guillaume, T.; Heard, D. E.; Lehman, J. H. J. Chem. Phys. 2024, 161 (9).

#B6: Atomic and molecular spectroscopy, photo-induced processes

Photoionisation, Rayleigh, and Raman scattering cross sections for the hydrogen molecule and its ion

Adam Singor¹; Liam Scarlett¹; Mark Zammit²; Igor Bray¹; Dmitry Fursa¹

¹ Curtin University

² Los Alamos National Laboratory

Photon scattering cross sections have proved essential in many applications, such as modelling opacities and radiative transport, studying the cooling of astrophysical plasma, analysing planetary atmospheres, and Raman spectroscopy.

In particular, Raman spectroscopy of H₂ plays an important role in analysing hydrogen storage techniques, monitoring ortho-to-para conversion, and monitoring nuclear waste.

Atomic and molecular hydrogen are abundant in the interstellar

medium, with H₂⁺ being formed by the radiative association of protons and atomic hydrogen, and ionisation of H₂.

Hence, photon scattering cross sections for H₂ and its ion are of particular interest in astrophysics.

Photon-molecule scattering processes have been well understood to second order in perturbation theory since the development of the Kramers-Heisenberg-Waller (KHW) matrix element [1,2] in the mid-1920s.

We have calculated photoionisation cross sections for all bound vibrational levels of the 1sσ_g ground electronic state of H₂⁺ and its isotopologues [3].

Rayleigh and Raman scattering cross sections have been calculated for transitions between all rovibrational levels of the X¹Σ_g⁺ ground electronic state of H₂, resulting in a total of 9582 Rayleigh and Raman cross sections [4].

This work represents the most comprehensive study of photon scattering on molecular hydrogen, and extends of our approach to photon scattering on atoms to diatomic molecules.

Isotopologue effects have been investigated and were found to be small.

Thermally-averaged photoionisation, Rayleigh, and Raman scattering cross sections have been produced for a system in local thermodynamic equilibrium.

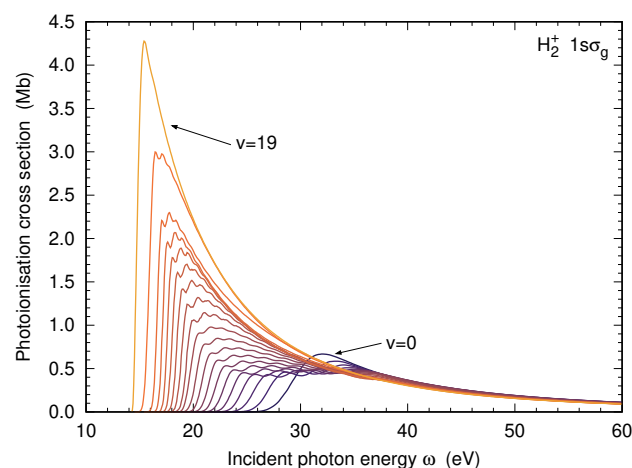


Fig.: Photoionisation cross sections for all bound vibrational levels of the 1sσ_g ground electronic state of H₂⁺ by unpolarised light.

[1] H. A. Kramers and W. Heisenberg, Z. Phys. **31**, 681 (1925).

[2] I. Waller, Z. Phys. **51**, 213 (1928).

[3] A. J. C. Singor, L. H. Scarlett, M. C. Zammit, I. Bray, and D. V. Fursa, ApJS **269**, 19 (2023).

[4] A. J. C. Singor, L. H. Scarlett, M. C. Zammit, I. Bray, and D. V. Fursa, J. Chem. Phys. **161**, 244304 (2024).

#B7: Atomic and molecular spectroscopy, photo-induced processes

Monochromatic source of ions and electrons for nanosciences

Clélia Bastelica¹; Azer Trimèche¹; Martin Schmidt²; Colin Lopez²; Matthieu Viteau³; Patrick Cheinet¹; Daniel Comparat¹; Yan J. Picard¹

¹ Université Paris-Saclay, CNRS, Laboratoire Aimé Cotton, 91405, Orsay, France.

² Université Paris-Saclay, CNRS, Ecole Normale Supérieure Paris-Saclay, CentraleSupélec, LuMin, Orsay, France

³ Orsay Physics, 95 Avenue des Monts Auréliens, 13710 Fuveau, France

Electron and ion beams have become indispensable tools in surface and material sciences, with an ever-increasing demand for higher resolution. This project aims to develop a Focused Ion Beam (FIB), called FIBback, leveraging two innovative concepts:

- A correlated source of ions and electrons, enabling, among other applications, complete trajectory control of the ion using information from its correlated electron [1, 2].

- A FIB (called ColdFIB) based on a cesium atom beam collimated by laser, excited to a Rydberg state, and then ionized by an electric field [3, 4].

We aim to enhance the resolution of ColdFIB through a novel and original approach: the spatial correlation. In fact, there is an existing correlation in position between the electron on its detector and the ion on the sample, both coming from the same atom. This correlation, added to the coincidence detection of the ion/electron pair provides informations about both correlated charged particles, which can be used to enhance the properties of the beam. Beam resolution will be improved either by utilizing real-time trajectory control of each ion [1], or through ghost imaging [2]. This new FIB prototype will also provide a deterministic ion source.

With this innovative FIB, we aim to achieve nanometer-scale resolution at low energy, paving the way for high-resolution, non-destructive imaging applications and deterministic implantation experiments.

References

- [1] C. Lopez, A. Trimeche, D. Comparat, and Y. Picard, *Physical Review Applied* 11, 064049 (2019).
- [2] A. Trimeche, C. Lopez, D. Comparat, and Y. Picard, *Physical Review Research* 2, 043295 (2020).
- [3] M. Reveillard et al., *Microscopy and Microanalysis* 24, 804 (2018).
- [4] M. Viteau et al., *Ultramicroscopy* 164, 70 (2016).

#B8: Atomic and molecular spectroscopy, photo-induced processes

High resolution spectroscopy of molecules confined in gas cells of sub-wavelength thickness

Hippolyte Mouhanna¹; Guadalupe Garcia Arellano¹; Joao Carlos de Aquino Carvalho²; Natalia de Melo³; Isabelle Maurin¹; Benoit Darquié¹; Athanasios Laliotis¹

¹ Université Sorbonne Paris Nord

² UFPE: Universidade Federal de Pernambuco

³ UFRPE: Universidade Federal Rural de Pernambuco

Miniaturized atomic vapor cells of nanometric thickness have become promising platforms for fundamental measurements, metrology and quantum technologies. For example, nanometric cells have been

used for exploring Dicke-type effects of confinement [1], measuring Casimir-Polder interactions, fabricating compact atomic clocks and probing collective effects. Extending these experiments to molecular gases is a fascinating prospect for applications in compact frequency referencing and for testing fundamental quantum electrodynamics using increasingly complex quantum objects. Towards this end, experiments have been performed with platforms such as hollow core fibers, tapered nanofibers and integrated waveguides. Moreover, selective reflection experiments with molecules have also been performed [2].

Here, we present our pioneering experiments probing molecular rovibrations of gases confined in micro-metric cells, whose thickness is comparable to the excitation wavelengths. We work in two distinct regions of the electromagnetic spectrum, probing v_1+v_3 resonances of acetylene at 1.530 μm , within the telecommunications wavelength range, as well as the v_3 and v_2 resonances of SF₆ and NH₃ respectively, in the mid-infrared fingerprint region around 10.55 μm . Thin-cell confinement allows us to explore and demonstrate Dicke-narrowing effects, probing molecules with linear sub-Doppler transmission spectroscopy. Our first experiment, reported recently in *Nature Communications* [3] uses a cell with a thickness that varies between 5.2-5.5 μm . This corresponds to $7\lambda/2$ and $\lambda/2$ thickness for acetylene and SF₆ or NH₃ rovibrations respectively. We also report measurements in a second cell of thickness ranging from 600-1200 nm allowing us to explore tighter molecular confinement. The transmission spectra displaying sub-Doppler characteristics due to the coherent Dicke narrowing are analyzed by means of a theoretical model [4] making specific assumptions about the physics and dynamics of confined molecules. In all the above measurements, the model reproduces exceptionally well the experimental data.

We focus our analysis on both the absolute signal amplitude and spectral lineshape. This allows us to confirm, within the limits of our precision, the hypotheses concerning the collisions with the cell-windows, the Maxwell-Boltzmann thermal distribution of velocities and the rotational redistribution (Boltzmann repartition function) of molecules after desorption from the wall. This is an important result, as the equilibrium conditions of confined gases have been put into question [5]. Furthermore, our analysis confirms that our spectroscopic technique can be used to determine molecular transition strengths and therefore enrich molecular databases. We demonstrate this by providing new data on the SF₆ greenhouse molecule for which databases are notoriously incomplete.

A major perspective resulting from this work is the measurement of Casimir-Polder interactions with molecules. For this purpose, we are currently building a new experiment to probe the strong HF rovibration at 2.5 μm . This experiment will allow us to probe strongly confined HF gas in a nanocell (100nm thickness) and measure the effects of molecular orientation in Casimir-Polder interactions.

References

- [1] G. Dutier et al., *Europhys. Lett.* EPL, 63, 35–41 (2003).
- [2] J. Lukusa Mudiayi et al., *Phys. Rev. Lett.*, 127, 043201 (2021).
- [3] G. Garcia Arellano et al., *Nat. Commun.*, 15, 1862 (2024).
- [4] G. Dutier, S. Saltiel, D. Bloch, M. Ducloy *J. Opt. Soc. Am. B*, 20, 793 (2003).
- [5] P. Todorov and D. Bloch, *J. Chem. Phys.*, 147, 194202 (2017).

#B9: Atomic and molecular spectroscopy, photo-induced processes

Comb-based Fourier-transform cavity-ringdown spectroscopy

Romain Dubroeuq¹; Dominik Charczun²;
Piotr Maslowski²; Lucile Rutkowski¹

¹ Université Rennes, CNRS, IPR (Institut de Physique de Rennes)-UMR 6251, F-35000 Rennes, France

² Institute of Physics, Nicolaus Copernicus University in Torun, Poland

Cavity-ringdown spectroscopy (CRDS) has become a cornerstone of modern spectroscopic techniques, known for its exceptional sensitivity and unique characteristics, such as calibration-free operation and immunity to light intensity fluctuations. These qualities result in highly accurate measurements of weak absorption lines. However, current continuous-wave (cw) laser-based methods require sequential acquisition of spectral elements, making experimental data more susceptible to time variations in temperature of the sample and generally taking longer to acquire. Consequently, there was a need in the scientific community to develop a broadband parallel acquisition method capable of providing multiplexed spectra with similar spectral resolution and absorption sensitivity.

The first demonstration of a broadband CRDS was conducted by Engeln and Meijer [1], using pulsed dye lasers and step-scan time-resolved Fourier transform spectrometers. However, limitations in resolution and acquisition time remained, prohibiting broader application. Thorpe et al. [2] later proposed employing an optical frequency comb as the light source for broadband CRDS, revisiting the spectral photography approach with enhanced sensitivity. In 2022, two new approaches were introduced to improve resolution and acquisition speed: combining CRDS with dual-comb interferometric detection [3] and time-resolved Fourier transform spectroscopy based on a single optical frequency comb [4]. A similar method was demonstrated in a recent paper by Liang et al. [5], with experiments performed directly in the mid-infrared range.

In this work, we present an approach based on direct frequency comb Fourier-transform, as introduced by Dubroeuq and Rutkowski [4], updated with recent developments [6]. Compared to the initial demonstration, a fundamental redesign of the frequency stabilization method has been made, enabling the extinction of comb light over a long duration without losing the comb-cavity lock. A cw-laser is introduced to act as an intermediary between the comb and the cavity.

The performance of the experimental setup is validated by high signal-to-noise ratio absorption spectra measurements of CO mixed with Ar over a broad coverage, confirming the influence of speed-dependent effects on the absorption line profiles.

References:

1. R. Engeln and G. Meijer Rev. Sci. Instrum. 67, 2708–2713 (1996).
2. M. J. Thorpe, K. D. Moll, R. J. Jones, B. Safdi, and J. Ye Science 311, 1595–1599 (2006).
3. D. Lisak, D. Charczun, A. Nishiyama, et al. Sci. Rep. 12, 2377 (2022).
4. R. Dubroeuq and L. Rutkowski Opt. Express 30, 13594–13602 (2022).
5. Q. Liang, A. Bisht, A. Scheck, P. G. Schunemann, and J. Ye, Nature 638, 941–948 (2025).
6. R. Dubroeuq, D. Charczun, P. Maslowski, L. Rutkowski APL Photon. 10, 026111 (2025).

#B10: Atomic and molecular spectroscopy, photo-induced processes

Chirality induced spin polarization in one-photon ionization by circularly polarized light

Philip Caesar Flores¹; Stefanos Carlstrom²; Serguei Patchkovskii²; Andres Felipe Ordonez³; Olga Smirnova²

¹ MaxMax-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany Born Institute

² Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin, Germany

³ Freie Universität Berlin

Geometric magnetism addresses the geometric origin of enantio-sensitive observables in one or multiphoton ionization from the emergence of the propensity field $\vec{B}_{\vec{k}}$ [1]. We extend this approach to spin-resolved one-photon ionization, i.e., $\vec{B}_{\vec{k},\mu} = i\vec{D}_{\vec{k},\mu}^* \times \vec{D}_{\vec{k},\mu}$, where $\vec{D}_{\vec{k},\mu}$ is the spin-resolved transition dipole with $\mu = \pm\frac{1}{2}$. Its respective net value on the energy shell (also known as *curvature*) is $\vec{\Omega}_{\mu} = \int d\Theta_k \vec{B}_{\vec{k},\mu}$, where $d\Theta_k$ corresponds to averaging over the orientations of photoelectron momentum $\vec{k}$ for fixed photoelectron energy $k^2/2$. It will be convenient to define the spin symmetric and antisymmetric vector quantities as follows: $\vec{A}_{\pm} = (\vec{A}_{\frac{1}{2}} \pm \vec{A}_{-\frac{1}{2}})/2$.

For one-photon ionization of an isotropic ensemble of chiral molecules by circularly polarized light $\vec{E} = E_{\omega}(\hat{x} + i\xi\hat{y})/\sqrt{2}$, we find that the enantio-sensitive orientation of a molecular cation $\vec{V}$ (e.g. permanent dipole) is locked to the spin of the detected electron $\hat{s}$. Specifically, the molecular vector orients itself along the direction orthogonal to both photoelectron spin $\hat{s}$ and photon spin $\hat{z}$:

$$\langle \vec{V} \rangle = \frac{\xi |E_{\omega}|^2}{12} [(\hat{\sigma}_{\frac{1}{2}} \times \vec{\Omega}_{-}) \cdot \vec{V}] (\hat{s} \times \hat{z}), \quad (1)$$

wherein the pseudoscalar $[(\hat{\sigma}_{\frac{1}{2}} \times \vec{\Omega}_{-}) \cdot \vec{V}]$ has opposite signs for opposite enantiomers. This suggests that if opposite enantiomers were oriented in the same way, then their spins would have opposite orientations, hence, equivalently oriented left and right enantiomers ionized by circularly polarized light should result in the ejection of photoelectrons with opposite spins – an effect which could be regarded as one of the manifestations of chirality induced spin selectivity [2].

We also show that the net photoelectron current acquires an enantio-sensitive component in the plane of polarization of light, i.e.,

$$\vec{j} = \vec{j}_0 + \left\{ \frac{\xi |E_{\omega}|^2}{12} \int d\Theta_k (\hat{\sigma}_{\frac{1}{2}} \cdot \vec{B}_{\vec{k},-}^{\perp}) \right\} (\hat{s} \times \hat{z}) \quad (2)$$

where, $\vec{j}_0$ is the PECD (photoelectron circular dichroism) current and $\vec{B}_{\vec{k},-}^{\perp} = \vec{k} \times \vec{B}_{\vec{k},-}$. The second term of $\vec{j}$ is a spin polarization vortex which rotates in opposite direction for opposite enantiomers. This observable arises from the “coupling” of the *propensity field* to spin, and can lead to high spin polarization even for very small spin-orbit interaction. This current reproduces earlier predictions of Ref. [3].

Our results are then illustrated for synthetic chiral matter. We construct chiral superpositions of electronic states in Argon, and perform *ab initio* simulations of its spin dynamics [4].

[1] A F Ordonez *et al.*, Comm Phys 6, 257 (2023).

[2] F Evers *et al.*, Adv Mater 34, 2106629 (2022).

[3] N A Cherepkov, J Phys B 16, 1543 (1983).

[4] S Carlström *et al.*, Phys Rev A 106 042806 (2022).

#B11: Atomic and molecular spectroscopy, photo-induced processes

Multi-platform theoretical calculations of oscillator strengths and transition probabilities in the Yb I isoelectronic sequence (Ta IV - Pt IX) for nuclear applications

Maxime Brasseur; Pascal Quinet; Patrick Palmeri

Université de Mons

All elements from rhenium to platinum will be produced in Tokamaks through neutron-induced transmutation of the tungsten which composed the divertor walls. Therefore, ionic impurities of all possible charge states should appear in the fusion plasma contributing to the power loss which does not make easy to get the self-maintained fusion reactions. However, the radiation emitted by these impurities will be useful for the plasma diagnosis (impurity influx, temperature and density). The identification of the spectral lines in experience and the knowledge of the radiative data for these ions is thus of great interest in this field. This work focuses on calculations of atomic structure, electric dipole transition probabilities and oscillator strengths for isoelectronic elements of Yb I from tantalum to platinum. A new set of electric dipole transitions from Ta IV to Pt IX are determined and listed using two independent methods, namely the pseudo-relativistic Hartree-Fock including core-polarization effects (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) approaches. The results from both methods are compared in order to assess the uncertainty and the quality of the new data.

#B12: Atomic and molecular spectroscopy, photo-induced processes

The interplay of bulk- and microviscosity effects on BODIPY-based molecular sensors

Stepas Toliautas; Domantas Narkevičius

Vilnius University, Faculty of Physics, Institute of Chemical Physics

Molecular compounds based on boron-dipyrromethene (BODIPY) have been shown to be promising candidates for microscopic, single-molecule scale sensing of environment properties, such as temperature or viscosity [1]. It is also possible to anchor the sensors to a specific type of microscopic environment, e.g. a lipid cell membrane, where the restricted molecular drift results in a measurable estimate of the bulk viscosity [2].

In this work, an existing quantum-chemical model of microviscosity sensitivity is applied to the snapshots of molecular dynamics simulations of a BODIPY sensor anchored in a bilayer lipid membrane. Intensity and timescales of the dynamic changes in expected microviscosity sensitivity are evaluated with the aim to determine how much the bulk drift (spanning 2-12 ns) influences the fluorescence lifetime-based viscosity measurements (0.1-5 ns).

Quantum-chemical computations were performed using resources at the supercomputer "VU HPC" of Vilnius University in the Faculty of Physics location.

[1] K. Maleckaitė et al., *Molecules* 27, 23 (2022)

[2] D. Narkevičius, master thesis, Vilnius University (2024)

#B13: Atomic and molecular spectroscopy, photo-induced processes

Towards deterministic ionization, loading, and sympathetic cooling of molecular ions for quantum logic spectroscopy

René Nardi¹; Brandon Furey²; Zhenlin Wu¹; Mariano Isaza Monsalve¹; Andrea Turci¹; Philipp Schindler¹

¹ Universität Innsbruck

² Universität Innsbruck

Quantum logic spectroscopy enables high-precision studies of molecular ions by using the controllability of co-trapped atomic ions. Molecular ions possess complex rovibrational structures that are challenging to probe directly. Instead, they can be sympathetically cooled and manipulated using atomic ions, allowing indirect measurements through shared motion in a trap. We present an experimental setup that utilizes time-of-flight mass spectrometry to identify molecular ion species produced via photoionization. Additionally, we perform detailed numerical simulations of the slowing, injection, and sympathetic cooling until the molecular ions form a stable configuration within a laser-cooled Ca⁺ ion string.

#B14: Atomic and molecular spectroscopy, photo-induced processes

Single and double ionization of pyridine and pyridine clusters

Sitanath Mondal¹; Brendan Wouterlood¹; Myriam Drissi¹; Gustavo A. Garcia²; Laurent Nahon²; Frank Stienkemeier¹; Sebastian Hartweg¹

¹ University of Freiburg

² Synchrotron SOLEI

Radiation damage on genetic materials is very important field of research. Photoionization studies of small biomolecular building blocks and their analogues can contribute by giving insights into energetics and dynamics of pathways of formation of secondary electrons and cationic dissociation reactions. Here, I present double imaging photoelectron photoion coincidence study of pyridine, pyridine clusters and pyridine water complexes. From our mass selected photoelectron spectra different fragmentation channels can be assigned to the corresponding cationic states. An additional analysis of electron-ion-ion coincidences allows us to obtain similar data for dicationic states of the molecules, revealing metastable decay channels and initial insights into stepwise dissociation pathways. For pyridine water complexes this approach allows to distinguish between different local and non-local double ionization mechanisms like Intermolecular Coulombic Decay (ICD).

#B15: Atomic and molecular spectroscopy, photo-induced processes

Internal decay processes in electron-rich symmetric dimer anions: An experimental probing using trapped ions in an Electrostatic ion-beam trap (EIBT)

Daniel Zajfman; Deepak Sharma; Oded Heber; Roby Chacko; Stav Knaffo

Weizmann Institute of Science, Israel

Understanding internal dynamics and decay processes is crucial in gas-phase molecular anion studies. Using our lab's unique facility[1], we investigated the long-timescale energy dynamics of Ag_2^- and Cu_2^- dimer anions. Internally hot anions from a Cesium sputter source are accelerated to 4.2 keV and stored in an Electrostatic Ion Beam Trap (EIBT). A laser-assisted velocity map imaging (VMI) spectrometer records ejected electrons, while a separate detector captures neutral counterparts. Coincidence data are analyzed over trapping time, and internal energy dynamics are inferred from photoelectron spectra (PES) at different storage windows. Experiments were conducted using 635 nm and 380 nm lasers.

The PES reveal intriguing results, including previously unreported peaks and differential decay rates for various transitions. We simulated spectra by computing Franck-Condon factors for all allowed transitions from the Ag_2^- ground electronic state to the Ag_2 ground electronic state. Calculations explain the spectral shape and indicate that faster-decaying transitions originate from higher rovibrational states.

Our results are compared with recent observations by Anderson et al. [2,3], who report spontaneous unimolecular decay of hot Ag_2^- and Cu_2^- dimer anions in the cryogenic DESIREE setup via fragmentation and electron emission. They attribute electron emission to vertical autodetachment (VAD) and fragmentation to tunneling dissociation, with the former showing a strong deviation from the BOA. However, their work does not provide any direct information on the internal energy distribution.

Our calculations rule out VAD and tunnelling dissociation as the cause for the faster decay of high rovibrational states. The origin of differential decay rates in the time dependent PES is still unclear. The experimental results and the possible causes for differential decay rates will be discussed at the conference.

We examine the possibility of non-BO transitions or excitation dependence of residual gas detachment. We pose the question whether the non-BO transitions in the case of electron-rich symmetric dimer anions are leading to radiative decay.

#B16: Atomic and molecular spectroscopy, photo-induced processes

Ground and First Excited States of the NaSr Molecule: Experimental and Theoretical Study

Jacek Szczepkowski¹; Marcin Gronowski²; Matylda Olko¹; Romain Vexiau³; Michał Tomza²; Olivier Dulieu³; Paweł Kowalczyk⁴; Włodzimierz Jastrzebski¹

¹ Institute of Physics Polish Academy of Sciences

² Institute of Theoretical Physics, Faculty of Physics, University of Warsaw

³ Laboratoire Aimé Cotton, CNRS, Université Paris-Saclay

⁴ Institute of Experimental Physics, Faculty of Physics, University of Warsaw

In recent years, a growing interest towards open-shell heteronuclear molecules can be noticed. These molecules attract particular attention of physicists involved in experiments at ultracold conditions, because they are known as “doubly polar molecules” having both electric and magnetic permanent dipole moments. Such properties provide a unique possibility for quantum control and simulations.

We report the first spectroscopic investigation of the NaSr molecule. Spectra related to the $\text{B}(2)^2\Sigma^+ \rightarrow \text{X}(1)^2\Sigma^+$ transition were observed with partial rotational resolution by thermoluminescence and laser induced fluorescence techniques. Simultaneously, potential energy curves of the lowest electronic states of NaSr and transition dipole moments were calculated using two different theoretical approaches. Comparison with theoretical results allowed to interpret the experimental spectra and deduce the salient molecular constants of the $\text{X}(1)^2\Sigma^+$ and $\text{B}(2)^2\Sigma^+$ states.

#B17: Atomic and molecular spectroscopy, photo-induced processes

Spectroscopic Studies of Cold, Trapped Negative Ions in Radiofrequency Multipole Traps

Sruthi Purushu Melath¹; Michael Philipp Hauck¹; Christine Lochmann¹; Robert Johannes Wild¹; Katrin Erath-Dulitz¹; Dasarath Swaraj¹; Franziska Dahlmann²; Marius Gerlach³; Dennis F. Dinu¹; Pavol Jusko⁴; Klaus R. Liedl¹; Stephan Schlemmer⁵; Sandra Brünken⁶; Roland Wester¹

¹ Universität Innsbruck

² KTH Royal Institute of Technology, Sweden

³ Radboud University

⁴ Max Planck Institute for Extraterrestrial Physics, Garching

⁵ University of Cologne

⁶ FELIX Laboratory Radboud University

Photodetachment spectroscopy is a powerful spectroscopic technique for determining the internal state distribution of a molecular anion. Previously, our group studied the threshold photodetachment spectroscopy of CN^- at both 16 K and 295 K in a 22-pole ion trap and measured the electron affinity of CN with great precision (EA: 3.864(2) eV) [1]. Here, we present results from our recent study of threshold photodetachment spectroscopy of C_2^- in a radiofrequency 16-pole ion trap at two different trap temperatures, 8 K and 150 K. We investigated the behavior of the cross section near the threshold for the ground-state transition, $\text{C}_2 \text{X}^1\Sigma_g^+ \leftarrow \text{C}_2^- \text{X}^2\Sigma_g^+$, and the excited state transition $\text{C}_2 \text{a}^3\Pi_u \leftarrow \text{C}_2^- \text{X}^2\Sigma_g^+$, which are expected to show p-wave

detachment and s-wave detachment behavior, respectively. By fitting the near-threshold behavior, we obtain precise values for the electron affinity of C_2 .

We also present our results from infrared predissociation (IRPD) spectroscopy of C_2H^- tagged with H_2 and D_2 , measured in the 350–3000 cm^{-1} range using the FELIX free-electron laser facility. Our experimental results, together with theoretical calculations, confirm the fundamental CCH bending, CC stretching, and the overtone of the CCH bending mode of the C_2H^- ion and D_2 stretching mode associated with the $C_2H^-D_2$ complex. Additionally, two spectral features observed in the 700–900 cm^{-1} region are most likely due to intermolecular interactions with the H_2 tag.

[1]. M. Simpson et al., J. Chem. Phys. 153, 184309 (2020).

#B18: Atomic and molecular spectroscopy, photo-induced processes

High-Fidelity Individual Addressing of Single Atoms in Quantum Registers at Three-Photon Laser Excitation of Rydberg States

Nikolai N. Bezuglov¹; Ilya I. Beterov²; Artūrs Ciniņš³; Kaspars Mičulis⁴; Elena A. Yakshina²; Pavel I. Betleni²; Ghadeer Suliman²; Denis B. Tretyakov²; Vasilii M. Entin⁵; Igor I. Ryabtsev²

¹ (1) Saint-Petersburg State University, 199034 Saint-Petersburg, Russia; (2) Rzhzanov Institute of Semiconductor Physics SB RAS, 630090 Novosibirsk, Russia

² (1) Rzhzanov Institute of Semiconductor Physics SB RAS, 630090 Novosibirsk, Russia; (2) Novosibirsk State University, 630090 Novosibirsk, Russia

³ University of Latvia, Faculty of Science and Technology, Institute of Atomic Physics and Spectroscopy, LV-1004, Riga, Latvia

⁴ (1) University of Latvia, Faculty of Science and Technology, Institute of Atomic Physics and Spectroscopy, LV-1004, Riga, Latvia; (2) National Research Nuclear University MEPhI, Moscow, 115409 Russia

⁵ Rzhzanov Institute of Semiconductor Physics SB RAS, 630090 Novosibirsk, Russia

Precise individual addressing of single atoms in quantum registers formed by optical dipole trap arrays is essential to achieve high-fidelity quantum gates in neutral-atom quantum computers and simulators. Two-qubit quantum gates are typically realized using coherent two-photon laser excitation of atoms to strongly interacting Rydberg states [1]. However, two-photon excitation encounters challenges in individual addressing with tightly focused laser beams due to atom position uncertainty and the spatial inhomogeneity in both Rabi frequencies and light shifts [2,3]. We numerically and analytically demonstrate that the fidelity of individual addressing can be improved by employing coherent three-photon laser excitation of Rydberg states [4]. For a specific example of $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow 6S_{1/2} \rightarrow nP$ excitation in ^{87}Rb atoms, we find that upon strong laser coupling in the second step (Rabi frequency Ω_2) and moderate coupling in the first and third steps (Rabi frequencies Ω_1 and Ω_3), the three-photon Rabi frequency is given by $\Omega = \Omega_1\Omega_3/\Omega_2$. If the spatial distributions of $(\Omega_1\Omega_3)$ and Ω_2 are arranged to be identical, Ω becomes independent of atom position, even within very tightly focused laser beams.

Figure (a) shows numerically (circles) and analytically (blue curve) calculated spatially-averaged amplitude A_1 of the first Rabi oscillation at three-photon excitation $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow 6S_{1/2} \rightarrow 70P_{3/2}$ in ^{87}Rb atoms. The A_1 -dependence on the “coverage” parameter w/a is given by the relation between laser spot radius w and atom position uncertainty a . A fairly good agreement is observed for $w/a \geq 2$. Figure (b) shows a comparison of numerically calculated spatially-averaged amplitudes of the first Rabi oscillation at three-photon excitation $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow 6S_{1/2} \rightarrow 70P_{3/2}$ and two-photon excitation

$5S_{1/2} \rightarrow 6P_{3/2} \rightarrow 70S_{1/2} \rightarrow 70P_{3/2}$ in ^{87}Rb atoms (with parameters taken from Ref.[1]). The three-photon excitation is almost unaffected by w/a variation even at $w/a = 2$, while for two-photon excitation the amplitude strongly decreases starting from $w/a = 5$.

Our approach can dramatically improve individual addressing of Rydberg excitation for neighboring atoms in trap arrays compared to conventional two-photon excitation schemes. Our findings are crucial for large-scale quantum registers of neutral atoms, where distances between adjacent atoms should be minimized to ensure stronger Rydberg interactions and compact arrangement of atom arrays.

Authors N.N.B., I.I.B., and I.I.R. acknowledge the support of the grant No. 23-12-00067 (<https://rscf.ru/project/23-12-00067/>) by the Russian Science Foundation. Author A.C. acknowledges the support of Latvian Council of Science project No. lzp-2023/1-0199.

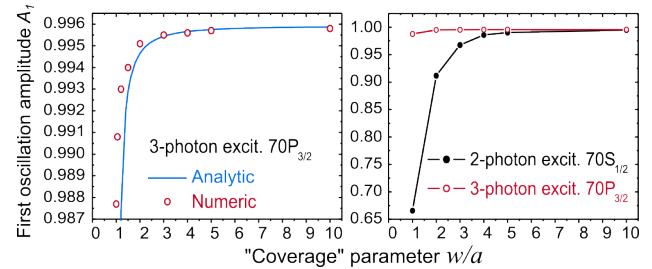


Fig.: (a) Numerically (circles) and analytically (blue curve) calculated spatially-averaged amplitude of the first Rabi oscillation at three-photon excitation $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow 6S_{1/2} \rightarrow 70P_{3/2}$ in ^{87}Rb atoms at large second-step Rabi frequency $\Omega_2/(2\pi) = 4 GHz$ and modest first-step and third-step Rabi frequencies $\Omega_1/(2\pi) = \Omega_3/(2\pi) = 126.5 MHz$. (b) Comparison of numerically calculated spatially-averaged amplitudes of the first Rabi oscillation at three-photon excitation $5S_{1/2} \rightarrow 5P_{3/2} \rightarrow 6S_{1/2} \rightarrow 70P_{3/2}$ with the above parameters and two-photon excitation $5S_{1/2} \rightarrow 6P_{3/2} \rightarrow 70S_{1/2} \rightarrow 70P_{3/2}$ at first-step detuning $\delta_1/(2\pi) = 1 GHz$ and first-step $\Omega_1/(2\pi) = 160 MHz$ and second-step $\Omega_2/(2\pi) = 50 MHz$ Rabi frequencies, as used in Ref.[1].

[1] H.Levine et al., Phys. Rev. Lett. 123, 170503 (2019).

[2] M.Saffman, J. Phys. B 49, 202001 (2016).

[3] S. de Léséleuc et al., Phys. Rev. A 97, 053803 (2018).

[4] N.N.Bezuglov et al., arXiv: 2411.06607 (2024).

#B19: Atomic and molecular spectroscopy, photo-induced processes

Electron Diffraction Imaging of Molecules via Ionization by Compton Scattering

A. Kügler¹; A. Pier¹; D. M. Haubenreißer²; F. Trinter³; I. Dwojak¹; J. Drnec⁴; J. Kruse¹; J. Stindl¹; L. Kaiser¹; L. Nowak¹; L. Ph. H. Schmidt¹; L. Sommerlad¹; M. Kircher¹; M. S. Schöffler¹; M. Schmidt¹; N. Anders¹; N. M. Novikovskiy²; N. Melzer¹; O. D. McGinnis¹; Philipp Demekhin²; R. Dörner¹; T. Jahnke⁵

¹ Institut für Kernphysik, Goethe-Universität Frankfurt, Germany

² Institut für Physik und CINSaT, Universität Kassel, Germany

³ Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

⁴ ESRF, The European Synchrotron, Grenoble Cedex 9, France

⁵ Max-Planck-Institut für Kernphysik, Heidelberg, Germany; European XFEL, Schenefeld, Germany

Compton scattering is the fundamental light-matter interaction pro-

cess discussed in the textbooks as a billiard-type collision, in which a photon (as a particle) is deflected and transfers parts of its energy and momentum to an electron initially at rest. If electron is bound in an atom or molecule, its momentum distribution contributes to the balance, which is known as the impulse approximation [1]. As a consequence, the momentum distribution of direct Compton electrons is given by the Fourier transform of the initial orbital displaced by the photon momentum transfer. Recent experimental and theoretical studies [2,3] highlighted the need to go beyond this approximation. In particular, Ref. [2] reported a backward scattering of the direct Compton electrons with respect to the photon momentum transfer and a simultaneous forward kick of the parent nucleus, while Ref. [3] demonstrated a scattering of the direct Compton electrons to all angles and a Coulomb focusing of the electrons by the ionization potential of the ion.

In the present work, we consider theoretically and experimentally the K-shell ionization of C and O atoms in carbon monoxide molecules by Compton scattering of 20 keV photons and report differential electron momentum distributions [4]. We observe diffraction patterns in the momentum distributions, which persist after integration over magnitudes and orientations of the photon momentum transfer in the frame of molecular reference. This phenomenon relies on the interference of the direct Compton electrons and those which are scattered on the parent and neighboring nuclei. The double-slit interference patterns in the electron momentum distribution can directly be related to the molecular orientation and the internuclear distance. The present results suggest that the imaging techniques, widely employed in the optical regime via laser-induced diffraction and soft x-ray domain via one-photon inner-shell photoionization, can be extended to the hard X-ray domain, where the photoionization is strongly suppressed, and the ionization by Compton scattering became dominant.

- [1] J. W. M. Du Mond, Phys. Rev. 33, 643 (1929).
- [2] M. Kircher et al., Nat. Phys. 16, 756 (2020).
- [3] N. Melzer et al., Phys. Rev. Lett. 133, 183002 (2024).
- [4] D. M. Haubenreißer et al, (2025) submitted

#B20: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

The features of binding of two multi-charged meso-porphyrins to nucleic acids

Olga Ryazanova

Department of Molecular Biophysics, B.Verkin Institute for Low Temperature Physics & Engineering of NAS of Ukraine

TMPyP4 is well-known *meso*-substituted porphyrin with high biological activity and unique spectroscopic and photophysical properties. This highly symmetric (D_{2h}) fluorescent compound is widely used as a photosensitizer in anticancer PDT, anti-viral and antimicrobial agent, an efficient probe for the nucleic acids structure and dynamics, a carrier of antisense oligonucleotides for their delivery, stabilizer of G-quadruplexes etc. The binding of TMPyP4 and its tricationic derivative to synthetic nucleic acids of different structure and base composition have been comprehensively studied by many authors and us [1–5] in a wide range of phosphate/dye ratio (*P/D*) using various spectroscopic methods. It was shown that the way of the porphyrin binding depends on NA base composition and spatial structure, and on *P/D*. An aggregation of both porphyrins on the biopolymers surface at a near-stoichiometric in charge *P/D* ratio has been revealed for all systems studied. The work is focused on comparison of our data with that of other authors on the spectroscopic features of the porphyrin binding to synthetic nucleic acids, their analysis and generalization.

References

- [1] O. Ryazanova, I. Voloshin et al, J. Fluoresc. doi:10.1007/s10895-024-04000-4 (2024).
- [2] O. Ryazanova, I. Voloshin et al, Mol. Cryst. Liq. Cryst. 698(1), 26 (2020).

[3] O. Ryazanova, V. Zozulya et al, Methods Appl. Fluoresc. 4(3), 034005 (2016).

[4] V. Zozulya, O. Ryazanova et al, Biophys. Chem. 185(1), 39 (2014).

[5] V. Zozulya, O. Ryazanova et al, J. Fluoresc. 20(3), 695 (2010).

Acknowledgements: The author acknowledges the National Academy of Sciences of Ukraine for the financial support (Grant No. 0123U100628) and Wolfgang Pauli Institute (Vienna, Austria) for Pauli Postdoc research training scholarships “Data analysis in molecular biophysics” 2021/22.

#B21: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Highly oriented pyrolytic graphite chemical bonding structure after gallium implantation

Tasabeeh Jafer¹; Hesham Abdelbagi²; Tőkési Károly³; Johan Malherbe¹

¹ University of Pretoria

² University of Zululand

³ HUN-REN Institute for Nuclear Research

Highly oriented pyrolytic graphite (HOPG) structural changes caused by gallium (Ga) implantation at room temperature were investigated. Raman spectroscopy was used to investigate the structural changes in HOPG after Ga implantation at different energies (i.e., 10, 20 and 30 keV) and fluences (i.e., 2×10^{15} , 5×10^{15} , 1×10^{16} , 2×10^{16} , 4×10^{16} , 5×10^{16} cm⁻²). SRIM (Stopping and Range of Ions in Matter 2013) software was used to determine the depth profiles of Ga ions and the degree of damage to HOPG (in dpa - displacement per atom) after implantation. The implantation was done at room temperature. SRIM predicted that implanting Ga into HOPG at 30 keV and at a fluence of 5×10^{16} cm⁻² created 100 dpa at a depth 15 nm below the surface. This indicates that HOPG structure becomes amorphous under this implantation detail. This also agrees with the Raman results, where HOPG characteristics D and G peaks at 1359 cm⁻¹ and 1582 cm⁻¹, respectively, have merged into a broad peak indicating the amorphisation of HOPG after implantation with 30 keV Ga ions at 5×10^{16} cm⁻². On the other hand, comparing the dpa obtained from SRIM results with the Raman results, it is clear that the HOPG sample requires a dpa above 26 dpa to become amorphous, which is much higher than previously reported (0.20 dpa). This could be due to the significant proportion of perfectly formed graphite crystallites in our HOPG samples (as seen from Raman results of virgin HOPG), which require higher fluences to be fully damaged (i.e., to become amorphized).

#B22: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

The primary steps of ion solvation in helium nanodroplets

Albert Muñoz¹; Christian Engelbrecht Petersen²;
Constant Schouder³; Henrik Stapelfeldt⁴; Jeppe
Christensen¹; Manuel Barranco⁵; Marti Pi⁵;
Simon Høgh Albrechtsen¹

¹ Department of Chemistry, Aarhus University

² Aarhus University, Department of Physics and Astronomy

³ ISMO, CNRS, Université Paris-Saclay

⁴ Aarhus University, Department of Chemistry

⁵ Departament FQA, Facultat de Física, Universitat de Barcelona

We present experimental results on the solvation dynamics of a single alkali cation in liquid helium, measured with atomic resolution and with femtosecond time resolution [1-2].

A single Na, K or Li atom sitting in its equilibrium position on the surface of a He nanodroplet is ionized by a 50 fs laser pulse. Thereby, an alkali ion, Ak^+ , is introduced instantly to the liquid helium solvent from the gas phase. Hereafter, the Ak^+ ion will gradually pick up helium atoms to form a solvation complex, Ak^+He_n . After a time delay, a Xe atom, residing in the interior of the droplet, is ionized by a 50 fs probe pulse. The created Xe^+ ion pushes the Ak^+He_n complex away from the droplet, due to the internal Coulomb repulsion. The mass and velocity of all Ak^+He_n complexes are recorded by the combination of a Velocity Map Imaging (VMI) spectrometer and a Tpx3CAM detector.

We find that the distribution of attached helium atoms is Poissonian for the first few helium atoms. The first 3 helium atoms for Li^+ , the first 5 atoms for Na^+ and the first 11 atoms for K^+ all attach at a constant rate of 1.8 He/ps, in droplets containing 5200 helium atoms on average. This is in good agreement with TDDFT [1,3] and RPMD [4] simulations of the process. The time-dependent mean dissipated energy from the complexes to the droplet have also been extracted from the same measurement. Finally, a novel analysis of the detected Ak^+He_n kinetic energies provide droplet size resolution of the above results.

[1] Albrechtsen et. al., Nature, 2023, doi:10.1038/s41586-023-06593-5

[2] Albrechtsen et. al., JCP, 2025, accepted, preprint:arXiv:2502.11783

[3] García-Alfonso et. al., JCP, 2024, doi:10.1063/5.0205951

[4] Calvo, JCP, 2024, doi:10.1063/5.0230829

#B23: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Cryogenic single nanoparticle mass spectrometry

Björn Bastian; Kleopatra Papagrigoriou; Sophia C. Leippe; Knut R. Asmis

Universität Leipzig

Nanoparticle (NP) mass spectrometry in the gas phase is a unique way to characterize individual isolated particles and thus assess their intrinsic properties, NP-to-NP variability and structural evolution, e.g. in studies on charging mechanisms [1], photophysics [2] or high

temperature reaction kinetics [3]. Our group focuses on cryogenic experiments to employ absorption spectroscopy, based on adsorption of messenger atoms or molecules on the NP surface and their desorption driven by laser heating with rates that are proportional to the absorption cross section [4]. An overview is given over the related goals, challenges and progress in charge state control, fluorescence thermometry [5] with the aim for temperature controlled experiments, and quantitative characterization of the adsorption on a NP surface.

[1] M. Grimm et al., Phys. Rev. Lett. 96, 066801 (2006)

[2] V. Dryza et al., Phys. Chem. Chem. Phys. 15, 20326 (2013)

[3] C. Y. Lau et al., J. Phys. Chem. C 127 (31), 15157 (2023)

[4] B. Hoffmann et al., J. Phys. Chem. Lett. 11, 6051 (2020)

[5] S. C. Leippe et al., J. Phys. Chem. C 128 (50), 21472 (2024)

#B24: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Collisional effects in the ultracold Rb-Hg system

Marcin Witkowski¹; Renu Bala¹; Adam Linek¹; Piotr Zuchowski¹; Michal Zawada²; Paul Julienne³; Roman Ciurylo¹

¹ Nicolaus Copernicus University in Torun

² Nicolau Copernicus University in Torun

³ Joint Quantum Institute, University of Maryland and NIST

We report the results of theoretical studies for the dependence of collisional shift and width on isotopic mass in a Hg 1S0-3P0 clock transition perturbed by Rb atoms.

Our theoretical analysis uncovers isotopic dependencies over a temperature range from μK to K, highlighting specific isotope pairs with minimal collisional effects, making them well-suited for two-species Rb-Hg composite atomic clock.

In this context, we explore the isotopic dependence of collisional line shape parameters, specifically the widths and shifts of the Hg clock transition, as influenced by Rb atoms within the temperature range up to 1K. To perform these calculations, we employed the Born-Oppenheimer effective interaction potential, incorporating the dominant long-range van der Waals terms. Our analysis reveals the relationship between the collisional line shape parameters and the reduced mass of the interacting atoms, as well as the variation of the scattering length in both the ground and excited states of the Hg-Rb system. Furthermore, we compare full quantum scattering calculations with a semiclassical approximation for collisional parameters.

#B25: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Measurement of atom-surface interactions in evanescent light filed by cold atomic fountain

Taro Mashimo; Masashi Abe; Satoshi Tojo

Department of Physics, Chuo University

Ultracold atomic cloud is one of highly sensitive tools to search for undiscovered field as a quantum sensor in the vicinity of a surface [1, 2]. We have investigated interactions between ultracold atoms and a

dielectric surface by an atomic fountain technique with moving an optical dipole trap beam. We initially loaded pre-cooled rubidium atoms to an optical dipole trap [3], and transported the atomic cloud with the temperature of 40 μK into a glass surface region by vertically changing the trap beam spatially. At the distance of 45 μm of the cloud from the glass surface, we suddenly turned off the trap beam with the initial velocity of 44 mm/s to generate the atomic fountain condition, and recaptured the atoms with experiences during their flights in the surface region in an evanescent light field near D2 line in the detuning range from -20 to +20 MHz. Thanks to the optical dipole and radiative forces near the resonance of the evanescent light, we derived slight differences of the numbers of recaptured atoms depending on the detuning. The differences are in good agreement with calculated results in the van der Waals and the Casimir-Polder potentials of the glass surface.

References:

- [1] Athanasios Laliotis, Bing-Sui Lu, Martial Ducloy, and David Wilkowski, *AVS Quantum Sci.* **3**, 043501 (2021).
- [2] Kosuke Shibata, Satoshi Tojo, and Daniel Bloch, *Optics Express* **25**, 9476 (2017).
- [3] Taro Mashimo, Masashi Abe, and Satoshi Tojo, *Phys. Rev. A* **100**, 064426 (2019).

#B26: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Excitations of a binary dipolar supersolid

Wyatt Kirkby¹; Au-Chen Lee²; Danny Baillie²; Tom Bland¹; Francesca Ferlaino¹; Blair Blakie²; Russell Bisset¹

¹ University of Innsbruck

² University of Otago

Supersolids are a remarkable state of matter, exhibiting both superfluidity and crystalline properties. We predict a rich excitation spectrum for a binary dipolar supersolid in a linear crystal geometry, where the ground state consists of two partially immiscible components forming alternating, interlocking domains. We identify three Goldstone branches, each exhibiting first-sound, second-sound, or spin-sound character. By analogy with a diatomic crystal, the resulting lattice has a two-domain primitive basis, and we find that the crystal (first-sound-like) branch splits into optical and acoustic phonons. Additionally, we identify a spin-Higgs branch associated with the supersolid modulation amplitude [1].

- [1] W. Kirkby, Au-Chen Lee, D. Baillie, T. Bland, F. Ferlaino, P. B. Blakie, R. N. Bisset, *Phys. Rev. Lett.* **133**, 103401 (2024)

#B27: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Dipole-Mode Spectrum and Hydrodynamic Crossover in a Resonantly Interacting Two-Species Fermion Mixture

Alberto Canali¹; Zhu-Xiong Ye²; Chun-Kit Wong³; Marian Kreyer⁴; Luc Absil¹; Emil Kirilov³; Rudolf Grimm⁴

¹ Institut für Experimentalphysik, Universität Innsbruck, Austria

² Institut für Experimentalphysik, Universität Innsbruck, Austria. State Key Laboratory of Quantum Optics Technologies and Devices, Institute of Opto-Electronics, Shanxi University, Taiyuan, 030006, China

³ Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria. Institut für Experimentalphysik, Universität Innsbruck, Austria

⁴ Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria

Ultracold quantum-gas mixtures of fermionic atoms with resonant control of interactions offer a unique test-bed to explore few- and many-body quantum states with unconventional properties. The emergence of such strongly correlated systems, as for instance symmetry-broken superfluids, is usually accompanied by hydrodynamic collective behavior. Thus, experimental progress in this field naturally requires a deep understanding of hydrodynamic regimes. We report on experiments employing a tunable Fermi-Fermi mixture of ¹⁶¹Dy and ⁴⁰K near quantum degeneracy. We investigate the full spectrum of dipole modes across a Feshbach resonance and characterize the crossover from collisionless to deep hydrodynamic behavior in measurements of frequencies and damping rates. We compare our results with theoretical models [1,2] that considers the motion of the mass centers of the two species and we identify the contributions of friction and mean-field interaction. We show that one oscillating mode exists over the whole range of interactions, exhibiting striking changes of frequency and damping in the deep hydrodynamic regime. We observe the second oscillating mode to split into two purely exponential damping modes. One of these exponential modes shows very fast damping, faster than any other relevant timescale, and is largely insensitive against experimental imperfections. It provides an accurate measure for the interspecies drag effect, which generalizes the concept of spin drag explored in other experiments [3,4]. We characterize the interspecies drag locally in terms of a microscopic friction coefficient and we discuss its unitarity-limited universal behavior on top of the resonance.

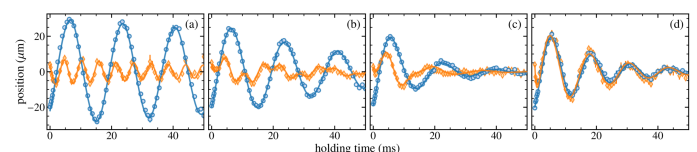


Fig.: Center-of-mass oscillations of the Dy (blue) and K (orange) clouds for increasing interaction strength. (a) Non interacting case, independent oscillations of the two clouds. (b,c) For intermediate friction increasing interaction effects are observed. (d) On resonance the interspecies interaction results in a locked hydrodynamic motion of both components.

- [1] S. Chiacchiera, T. Macrì, and A. Trombettoni, *Phys. Rev. A* **81**, 033624 (2010).

- [2] Y. Asano, S. Watabe, and T. Nikuni, *Phys. Rev. A* **101**, 013611 (2020).

- [3] A. Sommer, M. Ku, G. Roati, and M. W. Zwierlein, *Nature (London)* **472**, 201 (2011).

- [4] G. Valtolina, F. Scazza, A. Amico, A. Burchianti, A. Recati, T. Enss, M. Inguscio, M. Zaccanti, and G. Roati, *Nat. Phys.* **13**, 704 (2017).

#B28: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Dynamical quasicondensation in the weakly interacting Fermi-Hubbard model

Iva Brezinova¹; Stefan Donsa¹; Markus Stimpfle¹; Angel Rubio²

¹ Institute for Theoretical Physics, TU Wien

² Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science

Since the first pioneering experiments on signatures of superconductivity in laser-field driven materials [1], dynamical condensation effects have attracted a lot of experimental and theoretical interest. We theoretically study a related effect, i.e. fermionic condensation, in the paradigmatic Fermi-Hubbard model. Starting from a completely uncorrelated initial state, we show that upon expansion of the system in one dimension, dynamical (quasi)condensation occurs not only for large interactions via the condensation of doublons [2,3], but also for small interactions [4]. We address the question of whether the dynamical (quasi)condensation effect persists in the thermodynamic limit and in higher dimensions. For this purpose, we use the time-dependent two-particle reduced density matrix method [5], which allows the extension to large system sizes, long propagation times, and two-dimensional (2D) systems. Our results indicate that the effect vanishes in the thermodynamic limit. However, especially in 2D, further investigation beyond numerically tractable system sizes calls for the use of ultracold atom quantum simulators, for which we show that the described effect can be investigated by probing density fluctuations.

[1] D. Fausti et al., *Science* **331**, 189 (2011)

[2] M. Rigol et al., *Phys. Rev. Lett.* **93**, 230404 (2004)

[3] L. Vidmar et al., *Phys. Rev. X* **7**, 021012 (2017)

[4] I. Brezinová et al., *Phys. Rev. B* **109**, 174308 (2024)

[5] S. Donsa et al., *Phys. Rev. Research* **5**, 033022 (2023)

#B29: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

The moving Fermi polaron

Johanna Hennebichler¹; Ruben Erlenstedt¹; Erich Martin Dobler¹; Cosetta Baroni¹; Emil Kirilov²; Rudolf Grimm³

¹ IQOQI AG Grimm

² Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria. Institut für Experimentalphysik, Universität Innsbruck, Austria

³ Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria

Ultracold quantum gases offer a highly tunable platform for exploring strongly interacting many-body systems. In highly imbalanced mixtures, we can explore the quantum behavior of impurities. Our investigation focuses on bosonic ⁴¹K impurities interacting with a Fermi sea of ⁶Li atoms, forming a system that can be described in terms of quasiparticles known as Fermi polarons. While previous studies have probed the static and dynamic features of such polarons using radio-frequency spectroscopy [1], understanding kinetic properties such as effective mass and dispersion relation can be accomplished by means of Raman spectroscopy [2]. Notably, Raman transitions do not only facilitate manipulation of the impurity's internal state but they also offer control over its momentum state. Utilizing a newly built Raman setup, we can transfer multiple photon momenta to the impurities in a controlled manner, enabling the investigation of polaron behavior

with finite momentum within a Fermi sea. Here, we present our experimental results on the momentum-dependent polaron energy for different interaction strengths, highlighting the breakdown of the polaron picture at low momenta.

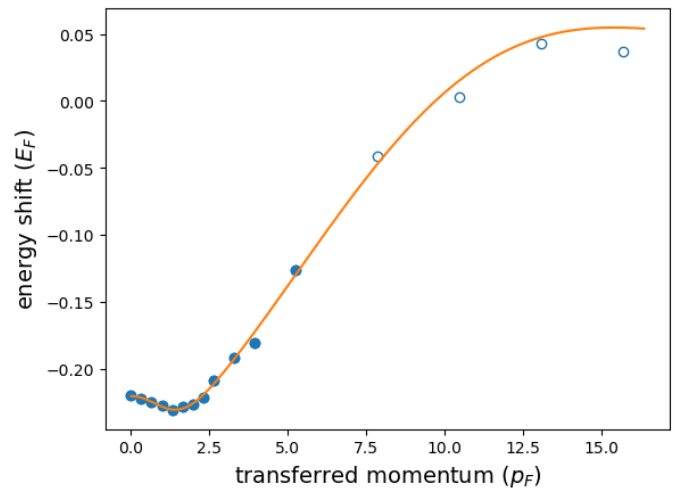


Fig.: The figure shows the energy of the attractive Fermi polaron as a function of the transferred momentum. The low-momentum behavior is governed by the effective mass, while at high momenta the polaron gets “undressed” and the effective mass description breaks down.

[1] Fritsche et al., *Phys. Rev. A* **103**, 053314 (2021)

[2] Ness et al., *Phys. Rev. X* **10**, 041019 (2020)

#B30: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Laser slowing of Aluminium-monofluoride in the deep ultraviolet

Lajos Palanki¹; Jionghao Cai¹; Carlos Alarcon-Robledo¹; Wei Wei Liu¹; Dylan Brown¹; Caleb Rich¹; José Eduardo Padilla-Castillo²; Russel Thomas²; Gerard Meijer²; Sidney Wright²; Stefan Truppe¹

¹ Imperial College London

² Fritz Haber Institute

In recent years, ultracold molecules have become a very promising platform for quantum information processing, studying quantum many-body physics and testing new physics beyond the Standard Model of particle physics.

Similar to alkaline earth (like) atoms (Yb, Sr, Cd) aluminium monofluoride (AlF), has a strong dipole-allowed transition (near 227.5 nm) to capture and cool a large number of molecules in a MOT and narrow spin-forbidden transitions for cooling to low temperatures in the μ K range. This might allow trapping laser-cooled molecules at high enough densities to study collisions between the molecules and evaporative cooling to form a degenerate gas of polar molecules.

We present a new laser system based on Vertical External Cavity Surface Emitting Lasers (VECSELs) to generate high-power DUV light for laser cooling. We show recent progress in slowing AlF from a buffer-gas source. We present simulations for expected capture properties of a MOT as well as future directions to improve slowing and UV light generation.

#B31: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Coherent control, state preparation and readout of polyatomic molecular ions via Quantum Logic Spectroscopy

Mariano Isaza Monsalve; Brandon Furey; Philipp Schindler; Rene Nardi; Zhenlin Wu

Universität Innsbruck

Molecular ions offer more degrees of freedom than atomic ions. These larger Hilbert spaces are rich and interesting landscapes to explore, possibly enabling quantum information applications such as quantum error correcting (QEC) schemes not available in atomic ions. This requires efficient and precise control of the molecular ion states. Co-trapping a molecular ion with an atomic ion facilitates state preparation and readout via quantum logic spectroscopy (QLS). We aim to use calcium-based molecules, e.g., CaH^+ or CaOH^+ , co-trapped with a 40Ca^+ ion for exploring these applications in QEC and precision spectroscopy. Coherent control within a rotational manifold of a molecular ion can be achieved by driving two-beam Raman transitions, as direct transitions between the Zeeman sublevels in the same manifold are forbidden by selection rules.

#B32: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Unitary Transformations using Robust Optimal Control on a Cold Atom Qudit

Eloi Flament¹; Nicolas Ombredane¹; Floriane Arrouas¹; Dominique Ronco¹; Bruno Peaudecerf¹; Dominique Sugny²; David Guéry-odellin¹

¹ LCAR, UT, CNRS

² Université Bourgogne Europe

In this research, we design and experimentally implement various robust quantum unitary transformations (gates) acting on d -dimensional vectors (qudits) by tuning a single control parameter using optimal control theory. The quantum state is represented by the momentum components of a Bose-Einstein condensate (BEC) placed in an optical lattice, with the lattice position varying over a fixed duration serving as the control parameter. To evaluate the quality of these transformations, we employ standard quantum process tomography. In addition, we show how controlled unitary transformations can be used to extend state stabilization to global stabilization within a controlled vector subspace. Finally, we apply them to state tomography, showing how the information about the relative phase between distant momentum components can be extracted by inducing an interference process.

#B33: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Spatially-resolved spin manipulation and readout of individual ultracold molecules in an optical lattice

Jonathan Mortlock; Adarsh Raghuram; Benjamin Maddox; Philip Gregory; Simon Cornish

Durham University

Creating arrays of ultracold molecules for quantum simulation of many-body systems is rapidly becoming a reality [1,2]. A key requirement for high-fidelity simulation of various spin models is the ability to simultaneously recover the population in each spin state. Using a series of manipulations proposed in [3], we experimentally demonstrate that two rotational states of ultracold RbCs molecules can be mapped to their constituent atoms: a molecule in the upper (lower) rotational state is detected as a Cs (Rb) atom in our imaging. We load a 2D optical lattice with over a thousand molecules and, by projecting an addressing tweezer, imprint a localized spin impurity by shielding a region of the gas from microwave excitation to the upper rotational state. Using optical microscopy, we then spatially resolve this impurity with single-molecule resolution while simultaneously imaging the rest of the gas in the other spin state.

[1] - Cornish, S. L., Tarbutt, M. R., & Hazzard, K. R. (2024). Quantum computation and quantum simulation with ultracold molecules. *Nature Physics*, 20(5), 730-740.

[2]- Christakis, L., Rosenberg, J. S., Raj, R., Chi, S., Morningstar, A., Huse, D. A., ... & Bakr, W. S. (2023). Probing site-resolved correlations in a spin system of ultracold molecules. *Nature*, 614(7946), 64-69.

[3] - Covey, J. P., De Marco, L., Acevedo, Ó. L., Rey, A. M., & Ye, J. (2018). An approach to spin-resolved molecular gas microscopy. *New Journal of Physics*, 20(4), 043031.

#B34: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Optical creation and manipulation of localised vortices in two-component Bose-Einstein condensates

Yakov Braver¹; Domantas Burba¹; Giedrius Žlabys²; Egidijus Anisimovas¹; Thomas Busch³; Gediminas Juzeliūnas¹

¹ Vilnius University

² Okinawa Institute of Science and Technology Graduate University

³ OIST Graduate University

Bose-Einstein condensates (BECs) provide a unique platform for studying quantum fluid dynamics, where macroscopic quantum phenomena such as superfluidity and quantised vortices emerge. Vortices in BECs are characterised by phase singularities in the condensate wave function, and they reveal insights into angular momentum quantisation and topological defects in quantum systems [1]. The study of vortices in degenerate bosonic and fermionic gases has broad implications, ranging from quantum turbulence [2] to connections with superconductivity and the structure of neutron stars [3].

A key challenge in the study of BEC vortices is their controlled creation and manipulation. Typically, the vortices are produced using optical

means: through phase imprinting [4], stirring with a laser beam [5], or using beams carrying orbital angular momentum, such as Laguerre–Gaussian (LG) beams [6]. Relatedly, an interesting playground for optical experiments is provided by the so-called Λ -type coupling configuration and the presence of a dark state. This optical coupling scheme has been used to, among others, realise atom control at subwavelength resolution [7], make narrow structures in the BEC [8], and to create vortices in BEC using Raman-type schemes [9].

In this work, we study the vortex states that emerge as a result of continuous interaction of a trapped two-component BEC mixture with the light fields in a Λ -type configuration. Specifically, we consider the case where one of the two beams is an LG beam, and investigate the resulting stationary states. The angular momentum of $\ell\hbar$ per photon carried by the LG beam leads to either one or both components being in a vortex state, with their vorticities differing by ℓ units. Depending on the ratio of magnitudes of the two beams, the ground state may have an unconventional structure, whereby the component having a vortex is surrounded by the second one which is vortex-free. The density profile of the vortex demonstrates a strong degree of localisation—away from the vortex core, the density falls off as $[1 + (\rho/a)^2]^{-1/2}$, where ρ is the distance from the core and a is a controllable parameter. Such a vortex can be moved around the trap by moving the laser beams. Provided the movement speed is less than approximately half the speed of sound in the condensate, the shape of the vortex retains its structure during the movement, and the density of the second component does not get distorted as well.

We support our findings with analytical arguments based on the approximate one-dimensional Gross–Pitaevskii equation (GPE) for the dark state, which features a geometric vector potential term. Additionally, we present numerical solutions of the full GPE system describing the Λ -coupled three-level system.

- [1] A. L. Fetter and A. A. Svidzinsky, *J. Phys.: Condens. Matter* **13**, R135 (2001)
- [2] M. Tsubota *et al.*, Takeuchi, *Phys. Rep.* **522**, 191 (2013)
- [3] P. Magierski *et al.*, *Eur. Phys. J. A* **60**, 186 (2024)
- [4] Ł. Dobrek *et al.*, *Phys. Rev. A* **60**, R3381 (1999)
- [5] K. W. Madison *et al.*, *Phys. Rev. Lett.* **84**, 806 (2000)
- [6] K.-P. Marzlin *et al.*, *Phys. Rev. Lett.* **79**, 4728 (1997)
- [7] A. V. Gorshkov *et al.*, *Phys. Rev. Lett.* **100**, 093005 (2008)
- [8] H. R. Hamedi *et al.*, *Opt. Express* **30**, 13915 (2022)
- [9] G. Nandi *et al.*, *Phys. Rev. A* **69**, 063606 (2004)

#B35: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Creation of ultracold Bosonic $^{39}\text{K}^{133}\text{Cs}$ Molecules in the rovibrational ground state

Charly Beulenkamp; Krzysztof Zamarski; Yi Zeng; Manuele Landini; Hanns-Christoph Nägerl

University of Innsbruck

The creation of ultracold heteronuclear molecules by assembly from precooled atoms has led to the realization of molecular gases with electric dipole-dipole interactions in the quantum degenerate regime [1,2], with exciting possibilities in the study of many-body dynamics, quantum computation and quantum simulation. One alkali molecule that has yet to be realized in the ultracold regime is KCs. It offers a dipole moment of 1.92 D, is chemically stable under collisions, and has both bosonic and fermionic isotopologues.

We report on the creation of a trapped sample of bosonic $^{39}\text{K}^{133}\text{Cs}$ molecules in their rovibronic ground state. We first describe our method for producing an ultracold mixture of ^{39}K and ^{133}Cs . Our cooling strategy is based on an established technique for ^{39}K [3], with modifications to allow sympathetic cooling of Cs. A narrow region of overlapping Feshbach resonances near 557G makes it possible to mix

and cool the two species close to the degenerate regime.

We then create up to 7500 weakly bound molecules at a temperature of 0.75 μK by magnetoassociation on an interspecies Feshbach resonance at 362G [4].

By means of one- and two-photon spectroscopy, and guided by predictions from theory [5], we have found and characterized an excited molecular state in the spin-orbit coupled $A^1\Sigma_0 - b^3\Pi$ potential with a narrow natural linewidth of $2\pi \times 80(6)$ kHz. Using this intermediate excited state, we perform stimulated Raman adiabatic passage to the rovibrational ground state with a one-way efficiency of 71%. Similar to other alkali molecule experiments, we observe a two-body decay with a loss coefficient in rough agreement with the predicted universal loss rate [6].

References

- [1] L. D. Marco *et al.*, *Science* **363**, 853 (2019).
- [2] N. Bigagli *et al.*, *Nature* **631**, 289–293 (2024).
- [3] M. Landini *et al.*, *PRA* **86**, 033421 (2012).
- [4] M. Gröbner *et al.*, *PRA* **95**, 022715 (2017).
- [5] D. Borsalino *et al.*, *J. Phys. B: At. Mol. Opt. Phys.* **49**, 055301 (2016).
- [6] P. S. Julienne *et al.*, *Phys. Chem. Chem. Phys.* **13**, 19114–19124 (2011).

#B36: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Density functional studies of vortices in rotating squeezed Bose-Bose mixtures

Ivan Poparić¹; Leandra Vranjes Markić¹; Jordi Boronat²

¹ University of Split, Faculty of Science

² Departament de Física, Universitat Politècnica de Catalunya

We investigate dilute Bose-Bose mixtures confined in an external harmonic potential that squeezes them in one spatial direction towards the two-dimensional limit, extending a recent study by some of the co-authors [1] by investigating rotating droplets which host vortices.

Specifically, we examine a quantum droplet composed of two hyperfine states of ^{39}K potassium atoms, utilizing Mean-Field and Lee-Huang-Yang interaction density functionals. We solve the extended Gross-Pitaevskii equation in the rotating frame of reference using imaginary time evolution to determine energies and density profiles. The stability of droplets is further confirmed by real-time evolution. Our analysis focuses on identifying the critical number of atoms required at which a central vortex becomes the ground state, for different magnetic fields, confinement strengths, and angular velocities. Additionally, we explore the optimal vorticity distribution across the mixture components for different atom numbers and angular velocities.

We find that the critical number of atoms needed to form a stable vortex decreases with the increase of squeezing. Through our investigation, we have discovered that for larger droplets and faster rotations, the vortex configuration maximizing angular momentum is favoured, while in smaller or slowly rotating droplets—where vortices are usually excited states—interactions become more significant.

- [1] A. Sanuy, *et al.*, *PRA* **109**, 013313 (2024).

#B37: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Prospects for Laser Cooling BN^-

Katrin Erath-Dulitz

Universität Innsbruck

Cold negative ions offer promising applications in areas such as quantum information science, fundamental physics, and chemistry. However, the cooling of these ions to temperatures near the Doppler limit has not yet been achieved.

Beyond ongoing work on the cooling of C_2^- , the boron nitride anion (BN^-) has emerged as a possible candidate ion for optical cycling and Doppler laser cooling. In our recent work [1], we investigated an optical cycling scheme for the Doppler cooling of cold, trapped $^{11}\text{B}^{14}\text{N}^-$ ions using excitation from the $X^2\Sigma^+$ ground state to the $B^2\Sigma^+$ excited state. Our results indicate that slow population decay via the first excited electronic state $A^2\Pi$ cannot be neglected. Consequently, various additional repump transitions, beyond what would be expected from the highly diagonal Franck Condon factor involving the $B^2\Sigma^+(v=0) \leftarrow X^2\Sigma^+(v=0)$ transition, must be excited to achieve efficient optical cycling. Furthermore, our findings indicate that the ions will likely need to be pre-cooled to translational temperatures near 1 K in order to reach a regime where Coulomb crystals are formed. For this reason, we have also performed extensive quantum calculations of potential energy curves for the interaction between BN^- and the potential cryogenic buffer gases He and Ar.

In addition to these theoretical results, I will present experimental progress towards the spectroscopic characterization of laser cooling transitions in BN^- .

[1] K. Dulitz et al., Phys. Scripta, accepted (2025). DOI: <https://doi.org/10.1088/1402-4896/adce43>

#B38: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Collective light scattering in an array of dysprosium atoms

Britton Hofer; Damien Bloch; Giulio Biagioni; Nathan Bonvalet; Antoine Browaeys; Igor Ferrier-Barbut

Institut d'Optique

Dissipative quantum many-body problems, such as those arising in collective light-matter interactions, present theoretical challenges. To explore these phenomena experimentally, we have developed an experimental setup that studies collective light scattering from an ordered ensemble of atoms. Recently, we achieved the first trapping and imaging of single dysprosium atoms in optical tweezers [1], extending the single-atom toolbox to lanthanides. Leveraging the rich internal structure of dysprosium, we can measure the atoms' internal states which we use to investigate collective dissipation both in the linear optics regime and at high saturation [2]. To further enhance the collective behavior of the atoms, we have two approaches. First, we cool the atoms close to their ground state using a 2 kHz transition [3]. Additionally, we are working to bring the atoms to a distance comparable to the wavelength of the transition used for light scattering by implementing a hybrid tweezer and accordion lattice setup.

[1] D. Bloch, B. Hofer, S. R. Cohen, A. Browaeys, and I. Ferrier-Barbut, *Trapping and imaging single dysprosium atoms in optical tweezer arrays*, Phys. Rev. Lett. 131, 203401 (2023)

[2] B. Hofer, D. Bloch, G. Biagioni, N. Bonvalet, A. Browaeys and

I. Ferrier-Barbut, *Single-atom resolved collective spectroscopy of a one-dimensional atomic array*, arXiv:2412.02541 (2024)

[3] G. Biagioni et al. *Narrow line cooling of single dysprosium atoms*, in preparation

#B39: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Self-Assembled Chains and Solids of Dipolar Atoms in a Multilayer

Grecia Guijarro¹; Gregory Astrakharchik¹; Giovanna Morigi²; Jordi Boronat Médico¹

¹ Universitat Politècnica de Catalunya

² Saarland University

We predict that ultracold bosonic dipolar gases, confined within a multilayer geometry, may undergo self-assembling processes, leading to the formation of chain gases and solids. These dipolar chains, with dipoles aligned across different layers, emerge at low densities and resemble phases observed in liquid crystals, such as nematic and smectic phases. We calculate the phase diagram using quantum Monte Carlo methods, introducing a newly devised trial wave function designed for describing the chain gas, where dipoles from different layers form chains without in-plane long-range order. We find gas, solid, and chain phases, along with quantum phase transitions between these states. Specifically, we predict the existence of quantum phase transitions from gaseous to self-ordered phases, as the interlayer distance is decreased. Remarkably, in the self-organized phases, the mean interparticle distance can significantly exceed the characteristic length of the interaction potential, yielding solids and chain gases with densities several orders of magnitude lower than those of conventional quantum solids.

[1] G. Guijarro, G. E. Astrakharchik, G. Morigi, and J. Boronat, Phys. Rev. Lett. 133, 233402 (2024).

#B40: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Towards highly polar CsAg and KAg ground state molecules

Jorge Mellado Muñoz; Jakub Pawlak; Om Tripathi; Jakub Dobosz; Mateusz Bocheński; Mariusz Semczuk

Institute of Experimental Physics, University of Warsaw, Warsaw, Poland

The creation of ultracold polar molecules has been actively pursued by many research groups. Up to now, these molecules have mainly composed of alkali dimers, limiting the maximum achievable permanent electric dipole moment to approximately 5.5 D (using LiCs). However, fully polarizing these molecular samples requires substantial electric fields of several kV/cm, presenting a technical challenge.

Here, we introduce first steps towards the production of ultracold CsAg and KAg molecules, which can achieve electric dipole moments nearing 10 D in the absolute ro-vibrational ground state. For CsAg, dipole moments exceeding 13 D can be attained in higher vibrational levels of the ground state potential, requiring only 0.3 kV/cm to fully polarize the sample.

The constructed setup will use two 2D MOTs as sources of pre-cooled atoms: one for potassium and cesium, and a separate one for silver.

This approach will avoid technical issues with coating the window opposing the silver atomic beam generated by the Zeeman slower and will result in a particularly compact vacuum system.

With enriched potassium dispensers and a versatile potassium laser system we have constructed, we will be able to switch between ^{39}K , ^{40}K , and ^{41}K , facilitating studies of both bosonic and fermionic KAg molecules.

We have performed high resolution, Doppler-free spectroscopy of molecular iodine at 656 nm to provide a frequency reference for a laser system that, after frequency doubling, delivers over 2 W of cooling light at 328 nm.

#B41: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

How rotation shapes the decay of diatomic carbon anions

Viviane C. Schmidt¹; Roman Čurík²; Milan Ončák³; Klaus Blaum⁴; Sebastian George⁴; Jürgen Göck⁴; Manfred Grieser⁴; Florian Grussie⁴; Claude Krantz⁴; Holger Kreckel⁴; Oldřich Novotný⁴; Kaija Spruck⁴; Andreas Wolf⁴

¹ Max-Planck-Institut für Kernphysik; Universität Innsbruck

² J. Heyrovsky Institute of Physical Chemistry

³ Universität Innsbruck

⁴ Max-Planck-Institut für Kernphysik

Molecules that are internally highly excited play an important role in a range of fields from atmospheric to plasma physics. Modelling such environments requires a detailed understanding of the molecules' behaviour at very strong excitations. However, this is a non-trivial task due to the high density of excited states as well as the variety of competing decay mechanisms available. The diatomic carbon anion C_2^- presents an excellent benchmark to understand the interplay of different decay channels at high internal excitation. The system is arguably the most extensively studied molecular anion in history. Yet, its decay behaviour at high internal excitation has long remained a riddle. When produced in a hot ion source, a subset of the resulting anions spontaneously eject their excess electron with a very narrow lifetime span of about 3 ms. While this autodetachment phenomenon has been known since the 1990s, the responsible anionic excited states and their decay mechanism have long remained elusive. Based on our measurements of autodecay of highly excited C_2^- at the Cryogenic Storage Ring (CSR) facility in Heidelberg, we carried out detailed calculations of the excited states and their decay behaviour [1,2]. Here, we were able to uncover the profound effect rotational excitation has on the system's electronic landscape, causing a reshuffling of the electronic states. This in turn alters the available decay channels at high excitations. The most severe example of this effect is visible in the lowest-lying electronic quartet state, $a^4\Sigma_u^+$. Here, a newly discovered autodetachment mechanism, rotationally assisted autodetachment, explains the feature measured at different ion storage facilities throughout the world over the last three decades.

[1] V. C. Schmidt et al., Phys. Rev. Lett. **133**, 183001, (2024)

[2] V. C. Schmidt et al., Phys. Rev. A **110**, 042828, (2024)

#B42: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Atomic cascade computations for astro and plasma physics

Stephan Fritzsche¹; Stefan Schippers²

¹ HI Jena

² Justus-Liebig-Universität Gießen, I. Physikalisches Institut

Atomic cascades occur frequently in Nature owing to the interaction of matter with particles and light. Such step-wise changes of an atomic and/or ionic ensemble are often "caused" by either the excitation of inner-shell electrons due to photon, electron, or particle impact, or by the capture of electron(s) into Rydberg orbitals as observed in many astrophysical environments [1].

In practice, most of these (atomic) cascades exhibit a rather high complexity, even if just the dominant decay paths are to be taken into account. This complexity arises first of all from the large number of decay paths that a (many-particle) quantum system may take. To systematically model such cascades, we have expanded JAC, the Jena Atomic Calculator [2], that supports the calculation of different atomic shell structures and processes. To model the excitation and subsequent decay of atoms and ions, we have classified and implemented a number of atomic cascade schemes [3] within the framework of JAC. These schemes include photo excitation and ionization, electron-impact excitation and ionization, various electron-capture cascades, or simply the efficient computation of associated plasma rate coefficients.

[1] S. Fritzsche, P. Palmeri and S. Schippers, Symmetry **13**, 520 (2021).

[2] S. Fritzsche, Comp. Phys. Commun. **240**, 1 (2019).

[3] S. Fritzsche et al., Eur. J. Phys. D **78**, 75 (2024).

#B43: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Angle-resolved spectroscopy of secondary electrons from surfaces emitted by highly charged ion impact

Anna Niggas¹; Daniel Thima¹; Filip Vuković¹; Victoria Vojtech¹; Matthias Werl¹; Jens Buck²; Kai Rossnagel²; Richard A. Wilhelm¹

¹ TU Wien

² Deutsches Elektronen-Synchrotron DESY

Secondary electron emission is one of the main energy dissipation channels of a highly charged ion impact on a material surface. While the electron yield, i.e. the number of electrons emitted per impacting ion, has been studied extensively for different ion velocities and charge states [1,2], literature on angle- and energy-resolved measurements of low-energy secondary electrons is scarce [3,4]. In particular, a momentum space image of emitted electrons through angle-resolved detection would clarify if the electrons are emitted isotropically from the ion itself or anisotropically from the solid surface through processes such as the interatomic Coulombic decay (ICD) [5].

We installed a small, portable electron beam ion source [6] at the ASPHERE III setup at DESY, which is equipped with a hemispherical energy analyser, allowing us to perform angle-resolved ion-induced electron emission spectroscopy (ARIIES). Our results show that the angular emission pattern depends on the electron yield: For singly-charged ions, the electron emission distribution resembles a cosine distribution, which flattens with increasing charge state. In other words, higher ion charge states result in increased total secondary electron

yields where emission to larger angles with respect to the surface normal is favoured. A possible explanation of this result is that space charge effects lead to the repulsion of electrons starting along the surface normal, which would only become relevant at high incident ion charge states where the electron yield increases. In this contribution, I will discuss these recent results and put them into context to show how this distortion of the electron emission spectrum may impact other experimental techniques.

- [1] H. Kurz *et al.*, *Phys. Rev. A* **49** 4693 (1994)
- [2] A. Niggas, J. Schwestka *et al.*, *Phys. Rev. Lett.* **129** 086802 (2022).
- [3] P. A. Zeijlmans van Emmichoven *et al.*, *Phys. Rev. A* **47** 3998 (1993).
- [4] H. Eder *et al.*, *Surf. Sci.* **472** 195 (2001).
- [5] R.A. Wilhelm *et al.*, *Phys. Rev. Lett.* **119** 103401 (2017)
- [6] D. Thima, A. Niggas *et al.*, *J. Phys. B: At. Mol. Opt. Phys.* **57** 165202 (2024).

#B44: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Does electron emission in highly charged ion collisions with surfaces occur above the surface or below?

Victoria Vojtech; Anna Niggas; Matthias Werl; Filip Vuković; Friedrich Aumayr; Richard Wilhelm

TU Wien

Slow highly charged ions (HCIs) exhibit interesting phenomena when interacting with a solid. For example, a single ion can induce nanometer-sized deformations on a surface [1] and lead to the emission of more than 100 electrons [2]. These effects result from the ion's large potential energy, ranging from tens to hundreds of keV [3], which is released within femtoseconds [4] upon impact. However, to harness the full potential of HCIs for technological applications, such as surface modification and analysis, a deeper understanding of the interaction processes is essential. Transmission experiments with free-standing 2D materials provide an ideal platform for such studies, as they allow us to isolate the surface-specific contributions in the HCI-solid interaction and provide insights into the timescales of the neutralization and energy deposition processes due to a limited interaction time with the solid material. Here, we focus on the emission of electrons as one of the main mechanisms for potential energy release. In particular, we want to tackle the question: from which side of the target are the electrons emitted?

To find the answer, we measured the electron emission induced by slow highly charged xenon ions (up to Xe³⁵⁺) transmitting through a freestanding single layer of graphene, for both the entrance and exit side, respectively. By detecting the emitted electrons in coincidence with the transmitted ion, we can relate the electron yield to specific ion impact parameters, energy loss and charge exchange. Preliminary results show that the electron yields are similar on both the entrance and exit side. If we look at the dependence of the electron yield on the number of electrons which the ion captures during the interaction, we find opposite trends on entrance and exit side. These measurements help us to unravel the complexity in HCI-surface collisions and to pinpoint the energy deposition process, timing and location.

References:

- [1] Schwestka, J. *et al.*, *ASC Nano* (2020), **14** 1936-0851
- [2] Schwestka, J. *et al.*, *J. Phys. Chem. Lett.* (2019), **10** 4805-4811
- [3] Gillaspay, J.D., *J. Phys. B: At. Mol. Opt. Phys.* (2001), **34** R93
- [4] Niggas, A. *et al.*, *Commun. Phys.* (2021), **4** 2399-3650

#B45: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electron collisions with liquid microjets: spectroscopy and reactivity

Juraj Fedor; Miloš Ranković; Samrat Saha; Hanns Ch. Schewe; Volodymyr Malynovskyy; Pamir Nag

J. Heyrovsky Institute of Physical Chemistry, Czech Academy of Sciences

Liquid microjet is a technique which enables bringing volatile liquids into the vacuum. It has been developed for the purpose of photoelectron spectroscopy which remains its most frequent use in laboratories world-wide. We have recently adapted this technique for probing collisions of free electrons with liquid interfaces.

I will present two main research directions on the electron collisions with the jets:

- Electron energy loss spectroscopy (EELS) is an approach for probing the excited states of the target. The incident electron energy is controlled and the outgoing (residual) energy is monitored, thus giving the information about energy levels of the target system. We recorded the EELS of liquid H₂O microjets under different conditions. The resulting spectra and their possible interpretation will be presented.
- Electron-induced reactivity. Here we irradiate the surface of a liquid with an electron beam of controlled energy and the macroscopic chemical changes in the samples are analyzed with various analytical techniques offline [1]. We have used detection techniques previously developed in radiation chemistry to: (i) scavenge the OH radicals in aqueous solutions with chemical dosimeters and (ii) use fluorescent spectroscopy to quantify the concentration of solvated electrons in the irradiated samples.

- [1] P. Nag *et al.* *J. Phys. B: At. Mol. Opt. Phys.* **56** (2023) 215201

#B46: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

State selective charge-exchange cross sections in collisions between Cq⁺ ions with sodium atoms

B.G. Csillag¹; D. Dunai¹; D. Nagy¹; D.I. Réfy¹; G. Anda¹; Karoly Tokesi²; M. Vécsei³; S. Zoletnik¹

¹ HUN-REN Centre for Energy Research, Budapest, Hungary

² HUN-REN Institute for Nuclear Research

³ Max Planck Institute für Plasmaphysik, Greifswald, Germany

The neutral alkali beams, such as lithium and sodium, were shown to be invaluable for measuring turbulence and electron density profiles in the boundary plasma [1]. These beams have also been proven to be useful for measuring local impurity properties using charge-exchange recombination spectroscopy [2]. The cross section calculations are vital to determine which spectral line can be significantly modulated by the charge-exchange (CX) processes between beam atoms and plasma ions.

In this work, the 3-body classical trajectory Monte Carlo (CTMC) method was used to determine the principal quantum number (*n*) and the orbital angular momentum quantum number (*l*) dependent CX cross sections for sodium atom and carbon ion collisions. The projectile carbon ion charge state was taken into account from the single charge till the fully stripped ion state. We performed the calculations

for 35 keV and 50 keV impact energies. The CTMC method is a non-perturbative method, based on the calculation of a large number of individual particle trajectories when the initial atomic states are chosen randomly [3-4]. In the present work, the CTMC simulations were made in the three-body approximation, where the many-electron target atom was replaced by a one-electron atom and the projectile ion was taken into account as one particle. The three particles are characterized by their masses and charges and Coulomb force is acting between the colliding particles. The effective charge of the target core was calculated according to the Slater's rules [5]. The initial conditions of the individual collisions are chosen at sufficiently large internuclear separations from the collision center, where the interactions among the particles are negligible. The classical equations of motion were integrated with respect to the time as independent variable by the standard Runge-Kutta method.

We found that higher the charge state higher value of n shows the maximum cross sections. In the similar fashion, for high n capture states the maximum l capture cross sections also shift toward to higher values of l . Moreover, we found that the CTMC modelling and the experiments on the alka-li beam of stellarator Wendelstein 7-X agree that for $q=6$ carbon ions the electron capture to the $n=8$ state occurs with the largest probability, while in case of the $q=5$ carbon ions the same holds for the $n=7$ states. The CTMC calculations indicate that in these cases the cross sections have a positive correlation with l .

This work has been carried out within the framework of the EUROfusion Consortium, funded by the European Union via the Euratom Research and Training Programme (Grant Agreement No 101052200 –EUROfusion). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Commission. Neither the European Union nor the European Commission can be held responsible for them.

References

- [1] S. Zoletnik et al., Rev. Sci. Instrum., 89 063503 (2018)
- [2] R.P Schorn et al., Nuclear Fusion, 32 351 (1992)
- [3] K. Tőkési and G. Hock, Nucl. Instrum. Meth., B 86 201 (1994)
- [4] K. Tőkési and Á. Kövér, J. Phys. B, 33 3067 (2000)

#B47: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Many-Body Theory Calculations of Positron Binding to Picolines

Tiarnan Smyth; Sarah Gregg; Dermot Green

Queen's University Belfast

Positron interactions with atoms and molecules are characterised by strong many-body correlations including polarisation of the electron cloud by the positron, screening of the electron-positron Coulomb interaction, and the process of virtual-positronium formation (in which a molecular electron temporarily tunnels to the positron) [1]. The correlations significantly enhance annihilation rates, modify scattering, and enable positron binding to atoms and molecules.

Recently our group developed an ab initio many-body theory approach to the calculation of positron binding in polyatomic molecules [1]. Here, we apply it to the picolines, the three isomers of methylpyridine (CH₃C₅H₄N).

Calculated positron binding energies and contact densities will be presented and compared to experiments where available. The role of the correlations, and the effect of the relative geometry of the nitrogen and methyl group will be examined.

- [1] J. Hofierka, ..., D. G. Green, Nature 606, 688 (2022).

#B48: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Experimental & theoretical cross sections for single & double ionization of open-4d-shell ions Xe¹²⁺ to Xe¹⁴⁺ by electron impact

Alexander Borovik¹; Alfred Müller¹; Benjamin Ebinger²; Fengtao Jin³; Michel Döhring²; Stefan Schippers⁴

¹ I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

² JLU Gießen

³ Department of Physics, National University of Defense Technology, 410073 Changsha, China

⁴ Justus-Liebig-Universität Gießen, I. Physikalisches Institut

Using the electron-ion crossed-beams technique, we have measured absolute cross sections for electron-impact single ionization of Xe¹²⁺ and Xe¹³⁺ ions, and double ionization of Xe¹²⁺, Xe¹³⁺, and Xe¹⁴⁺ ions. In addition we have performed corresponding calculations using a hybrid level-to-level and subconfiguration-average distorted wave approach. We find excellent agreement between our experimental and theoretical data except near the double-ionization threshold.

We present new experimental and theoretical cross sections for electron-impact single ionization of Xe¹²⁺ and Xe¹³⁺ ions, and double ionization of Xe¹²⁺, Xe¹³⁺, and Xe¹⁴⁺ ions [1]. The experiments were carried out by using the electron-ion crossed beams method with a recently commissioned electron gun, which extends our range of accessible electron energies from previously 1000 eV to now 3500 eV [3]. The calculations employed quantum mechanical perturbation theory in a hybrid approach [3,4], which augments fully-relativistic subconfiguration-averaged distorted-wave (SCADW) calculations with the more involved level-to-level distorted wave (LLDW) method for configurations straddling the ionization threshold. In the single-ionization calculations, we considered direct ionization (DI), excitation autoionization (EA), and resonant excitation double-autoionization (REDA), and, in the double ionization calculations, ionization autoionization (IA) and excitation double-autoionization (EDA). We find that, unlike in previous work [5,6], our theoretical cross sections agree with our experimental ones within the experimental uncertainties, except for the near-threshold double-ionization cross sections. We attribute this remaining discrepancy to the neglect of direct-double ionization in the present theoretical treatment.

References

- [1] Jin F et al. 2024 Eur. Phys. J. D 78 68
- [2] Ebinger B et al. 2017 Nucl. Instrum. Methods B 408 317
- [3] Jin F et al. 2020 J. Phys. B 53 175201
- [4] Jin F et al. 2020 J. Phys. B 53 175201
- [5] Pindzola M S et al. 2013 J. Phys. B 46 215202
- [6] Borovik Jr. A et al. 2015 J. Phys. B 48 035203

#B49: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Ternary association of H₃⁺ with H₂: effect of rotational excitation

Radek Plašil; Serhiy Rednyk; Petr Dohnal; Octavio E. Hernández Alvarez; Štěpán Roučka; Juraj Glosík

Charles University, Fac Math & Phys, Prague, Czechia

An association reaction of H₃⁺ ions with H₂ forming H₅⁺ was studied

in the temperature range of 15–35 K with either helium or hydrogen acting as a third body to understand the role of rotational excitation of colliding bodies.

A 22-pole radio-frequency ion trap apparatus [1] was employed to study the influence of the internal excitation of the reactants on the measured ternary reaction rate coefficient for H_3^+ formation. The population of the rotational ground state $J = 0$ of H_2 was varied from 25 % up to more than 99 % of all hydrogen molecules in these experiments. The measured values of the ternary reaction rate coefficients for $\text{H}_3^+ + \text{H}_2 + \text{H}_2$ association reaction are in agreement with the previously reported ion trap study by Paul [2]. The results indicate that the stability of the initial adduct formed in the collision of H_3^+ with H_2 is strongly dependent on the rotational state of the H_2 molecule. On the other hand, the character of the third body exerts little influence on the measured value of the ternary reaction rate coefficient.

[1] R. Plašil et al., *Astrophys. J.* **948**, 131, (2023)

[2] W. Paul et al., *Int. J. Mass Spectrom. Ion Processes* **149–150**, 373, (1995)

#B50: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Caesium photoionization for monochromatic electrons source for surface electron microscopy

Florent Vallée; Daniel Comparat

CNRS-LAC

By combining a monochromatic electron source and high performance detectors, we build with ISMO and SPEC a new electronic microscope call HREELM. This microscope enables the imaging and analysis of vibrational interactions on surfaces. Applications include nanophysics, nanochemistry and photonics.

KEY-WORDS : surface microscopy; pulse electron source ; Rydberg atoms

1. INTRODUCTION: MOTIVATION FOR BUILDING HREELM

For several decades now, we have been witnessing unprecedented development in the field of imaging and spectroscopy. Techniques are becoming increasingly sophisticated, pushing the limits of observation ever further. Nevertheless, each method has its advantages-and disadvantages.

Two methods of analysis can be distinguished: imaging and spectroscopic techniques. Imaging techniques include LEEM (Low-Energy Electron Microscopy), a full-field electron microscopy technique using low-energy electrons to image the sample surface. It can achieve a spatial resolution of 20 nm and a spectral resolution of 300 meV. For spectroscopic techniques, we can cite HREELS (High-Resolution Electron Energy Loss Spectroscopy), which is a spectroscopic technique based on the detection of inelastically scattered low-energy electrons. HREELS has a spatial resolution of 1 mm and a spectral resolution of 1 meV.

There is interest in the design of a new surface analysis instrument combining the features of LEEM and HREELS: HREELM (High-Resolution Electron Energy Loss Microscope). This is a full-field technique enabling simultaneous high-resolution imaging and spectroscopy. Resolution of phonons and surface plasmons requires an energy dispersion of less than 10 meV at a flux of 100 pA. Spatial resolution would be of the order of 10 nm [1].

1. DESCRIPTION DU SET UP EXPERIMENTAL

A) THE ELECTRONS SOURCE

A key aspect of HREELM design is the electron source used. It must be capable of achieving a flux in excess of 100 pA for good brilliance, with an energy dispersion of the order of 5-10 meV. To meet these criteria, Rydberg atom ionization was the obvious choice [2]. The entire source consists of a cesium jet, three lasers to excite the cesium atoms into a Rydberg state, and circular electrodes pierced at the center to create an electric field to

which the Rydberg atoms will be exposed.

In this situation, the energy dispersion of the source is given by the formula :

$$\Delta E = F \Delta z$$

With Δz the ionization zone imposed by the Rydberg resonance width and F the electric field imposed on the atoms.

B) ELECTRONS DETECTION SCHEME

Another important aspect of HREELM is the electron detection system. This is because the energy difference between electrons after their interaction with the sample will be small. A high-precision detection system is therefore required.

To achieve this, a time-of-flight measurement can be used. After interacting with the sample, the electrons are detected by a system of microchannel wafers coupled to a sensor which gives the position of the electrons and their arrival time on the sensor. In our case, we chose to use the Timepix 4, which is the only sensor capable of achieving the desired spatial and spectral resolution while supporting the flow of electrons imposed by the microchannel wafers.

However, to determine the time of flight, we need to know not only the arrival time of the particles, but also their departure time. So we use the electron/ion correlation to obtain the electron departure time.

3. RESULTS OBTAINED AND WORK IN PROGRESS

To be able to resolve phonons or molecular bonds, you need an electron source that meets all the above criteria. In order to test whether these criteria have been validated, it was necessary to build a first HREELM prototype.

The latter features an electron source based on ionization of Rydberg atoms and a detection system consisting of two microchannel wafers to amplify the electron flow, plus a phosphor screen to visualize the electron position. This device has proved that the three criteria can currently be achieved separately, but not simultaneously.

Current work consists in characterizing the electron source designed, in particular by studying the different Rydberg states, improving the detection system using Timepix, and working on the integration of all the elements of the experiment (time-of-flight tube, sensor, etc.).

#B51: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Experiments on Three-Body Association of Noble Gases in an RF Multipole Ion Trap

Michael Philipp Hauck; Robert Johannes Wild; Sruthi Purushu Melath; Roland Wester

Universität Innsbruck

Three-body association describes the process where three atoms or molecules collide to form a bound complex between two of them. This process plays a role in a multitude of physical systems, for example ozone formation in the atmosphere, the formation of clusters in supersonic jets, cold and ultracold chemistry and in tagging spectroscopy [1]. Ab initio calculations of three-body association reactions are still challenging and experimental data is needed as a benchmark for theoretical calculations. Three-body association reactions of noble gases have been previously studied using supersonic flow [2], but these measurements are limited by a fixed maximum interaction time in the order of milliseconds. This work aims to measure the reaction rate coefficient inside our cryogenic RF 16-pole wire trap, utilizing the long storage times that can be reached in our trap at lower temperatures [3]. Longer interaction times in turn mean the reaction can be observed at lower densities, which could allow us to measure the lifetime of the meta stable complex [4]. Our group has previously studied the three-body association of Cl^- with H_2 [5]. Additionally the three-body association rate coefficient for He is so well studied, by measuring it, we can extract the ion temperature in our trap [6].

[1] M. Mirahmadi and J. Pérez-Ríos, Three-Body Recombination in Physical Chemistry, *Int. Rev. Phys. Chem.* **41**, 233 (2022).

- [2] S. Hamon, et al., Low-Temperature Measurements of the Atomic Association Reaction $\text{Ar}^+ + 2\text{Ar} \rightarrow \text{Ar}_2^+ + \text{Ar}$, *Chem. Phys. Lett.* 288, 523 (1998).
- [3] C. Lochmann, et al., Three-Body Collisions Driving the Ion-Molecule Reaction $\text{C}_2^- + \text{H}_2$ at Low Temperatures, *J. Phys. Chem. A* 127, 4919 (2023).
- [4] I. Zymak, et al., Ternary Association of H^+ Ion with H_2 at 11 K, Experimental Study, *The European Physical Journal Applied Physics* 56, 24010 (2011).
- [5] R. Wild, et al., Complex Formation in Three-Body Reactions of Cl^- with H_2 , *J. Phys. Chem. A* 125, 8581 (2021).
- [6] R. Plašil, et al., Stabilization of $\text{H}^+ - \text{H}_2$ Collision Complexes between 11 and 28 K, *Phil. Trans. R. Soc. A* 370, 5066 (2012).

#B52: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Atomistic Computer Simulations of $\text{Fe}(\text{CO})_5$ Fragmentation Dynamics on a Substrate

Hlib Lyshchuk¹; Alexey Verkhovtsev²; Juraj Fedor³; Andrey Solov'yov²

¹ UCT Prague; J. Heyrovský Institute of Physical Chemistry CAS

² MBN Research Center gGmbH

³ J. Heyrovský Institute of Physical Chemistry CAS

We present the results of a computational study focusing on the radiation-induced fragmentation dynamics of $\text{Fe}(\text{CO})_5$ precursor molecules on experimentally relevant substrates. A combination of different computational methods is employed, including (i) quantum chemistry methods and (ii) the irradiation-driven molecular dynamics method [1] using the software package MBN Explorer [2]. Following the previous study of $\text{Fe}(\text{CO})_5$ fragmentation in the gas phase and in a cluster environment [3], this work extends the analysis to surface-bound conditions, taking into account the energy and momentum transfer between the molecule and the substrate. The role of the substrate in quenching bond dissociation events and suppressing molecular fragmentation is analyzed. Preliminary results are presented for two energy transfer mechanisms: a thermal mechanism, where excess kinetic energy is distributed among all atoms of the molecule, and a localized mechanism, where energy is deposited in a specific covalent bond [3,4]. In addition, the simulations provide detailed information on the kinetic energy evolution of intact $\text{Fe}(\text{CO})_5$ molecules and their fragments. These findings aim to deepen the atomistic understanding of the radiation-induced chemistry during focused electron beam induced nanofabrication with $\text{Fe}(\text{CO})_5$ and provide transferable insights for other precursors, such as MeCpPtMe_3 [4]. Ultimately, this research should contribute to the optimization of protocols for 3D nanoprinting of iron-based nanostructures for various technological applications.

Acknowledgments:

This work was supported from the grant of Specific university research –A2_FCHI_2025_037.

References:

- [1] G.B. Sushko, I.A. Solov'yov, and A.V. Solov'yov, *Eur. Phys. J. D* 70, 217, (2016)
- [2] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, and A.V. Solov'yov, *J. Comput. Chem.* 33, 2412, (2012)
- [3] B. Andreides, A.V. Verkhovtsev, J. Fedor, and A.V. Solov'yov, *J. Phys. Chem. A* 127, 3757, (2023)
- [4] H. Lyshchuk, A.V. Verkhovtsev, J. Kočíšek, J. Fedor, and A.V. Solov'yov, *J. Phys. Chem. A* 129, 2016, (2025)

#B53: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Dissociative electron attachment as a mechanism for formation of negative molecular ions in the interstellar medium

Elizabeth Aubin¹; Jean-Christophe Loison²; Mehdi Ayouz³; Viatcheslav Kokoouline¹

¹ University of Central Florida

² ISM, Université de Bordeaux

³ Université Paris-Saclay, CENTRALESUPÉLEC

Several negative molecular ions have been detected in the interstellar medium CN^- , C_3N^- , C_5N^- , C_7N^- , C_4H^- , C_6H^- , C_8H^- , C_{10}H^- . Since their discovery, for many years, there had been a general consensus in the community of modelers that in the interstellar medium (ISM) the ions are formed by the process of radiative electron attachment (REA). However, in several recent studies it has been shown that the REA process is too slow to explain the observed abundance of the ions in the ISM. In this study, we consider an alternative process of formation of ions: by dissociative electron attachment (DEA). First-principle calculations were performed to evaluate the cross sections and the rate coefficient for the DEA process to the HNCCC molecule, leading to formation of C_3N^- in the ISM. The obtained rate coefficient is large enough to explain the observed abundance of C_3N^- in the ISM. While no full calculations were performed for other molecular ions, observed in the ISM, it is expected that rate coefficients for their formation by similar reactions are also large enough to explain their formation in the ISM by DEA.

#B54: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

The Mutual Neutralization of Hydronium and Hydroxide.

Alon Bogot¹; Arnaud Dochain²; Daniel Strasser³; Henning Schmidt²; Henning Zettergren²; Mathias Poline²; MingChao Ji²; Richard Thomas²

¹ the Hebrew university of Jerusalem

² Stockholm University

³ Hebrew university of Jerusalem

The feasibility of performing merged beam experiments with trapped fast ion beams of molecular cations and anions at the double electrostatic storage ring (DESIREE) and the hybrid electrostatic ion beam trap (HEIBT), [1,2] opens new opportunities to study mutual neutralization reactions. Here, I will present our findings from merged beam experiments performed at DESIREE on the mutual neutralization of hydronium (H_3O^+) and hydroxide (OH^-), [3] and their isotopomers. [4] 3D coincidence imaging of the neutral products allowed us to disentangle the different competing proton-transfer and electron-transfer mechanisms. We identified a predominant e-transfer mechanism that forms either one or two OH radicals in a single neutralization reaction. By analyzing measured 3-body momentum correlations, we found that the distance at which the electron transfer occurs determines the final product channel. Electron transfer at a distance of $\sim 4\text{\AA}$ (left panel) forms the neutral H_3O radical intermediate ground state, which then dissociates into H_2O and H. In contrast, electron transfer at $\sim 10\text{\AA}$ presented in the right panel forms an electronically excited H_3O intermediate that dissociates into H_2 and a 2nd OH radical. These mutual neutralization dynamics of the isolated water ions can be related to ion-ion reactions on the liquid water surface and offer an explanation

for the recent observations of spontaneous hydrogen peroxide formation in pure water microdroplets.[5-7]

References

- [1] A. Bogot et al, Phys. Chem. Chem. Phys., 25, 25701-25710 (2023)
- [2] H.T. Schmidt et al, Rev. Sci. Instrum., 84, 055115 (2013)
- [3] A. Bogot et al, Science, 383, 285-289 (2024)
- [4] A. Bogot et al, preprint available at Research Square <https://doi.org/10.21203/rs.3.rs-4777257/v1>
- [5] J.K. Lee et al, PNAS, 116 (39), 19294-19298 (2019)
- [6] P. Skurski and J. Simons, J. Chem. Phys., 160, 034708 (2024)
- [7] J.P. Heindel et al, Nat Commun, 15, 3670 (2024)

#B55: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Attosecond magnetic pulses emerging from ring-current gates

Alba de las Heras¹; Franco P. Bonafé¹; Carlos Hernández-García²; Angel Rubio¹; Ofer Neufeld³

¹ Max Planck Institute for the Structure and Dynamics of Matter and Center for Free-Electron Laser Science

² Universidad de Salamanca

³ Technion - Israel Institute of Technology

We theoretically propose a method to synthesize the first attosecond magnetic pulses with tunable waveform [1]. Our ab initio calculations predict a magnetic pulse with a duration of 787 as and a high flux density of ~ 1 T at a few hundred nanometers from the source, paving the way for attosecond control and measurement of magnetization and chiral dynamics.

[1] A de las Heras et al., J. Phys. Chem. Lett. 14, 11160 (2023)

#B56: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Ionization-induced proton-transfer dynamics in formic acid dimer

Saroj Barik¹; Ester Livshits²; Roi Baer³; Daniel Strasser¹

¹ Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel

² Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel. Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

³ Institute of Chemistry, The Hebrew University of Jerusalem, Jerusalem 91904, Israel. Fritz Haber Research Center for Molecular Dynamics, The Hebrew University of Jerusalem, Jerusalem 9190401, Israel

A dimer system can undergo ultrafast symmetry breaking by charge localization upon ionization. Our recent work explored symmetry breaking dynamics in the Van der Waals bound CO_2 dimer using EUV pump - EUV probe Coulomb explosion imaging.[1] Here, I will present the symmetry breaking dynamics of a prototypical hydrogen bonded formic acid (FA) dimer. Similar to DNA base pairs, the FA dimer is bound by two hydrogen bonds, which form the ring-structure. Dimers in a neat FA molecular beam were probed by EUV pump- near IR probe 3D coincidence imaging. Transient enhancement of protonated formic acid cation signal with 150 fs lifetime was observed. Ab initio molecular dynamics simulations predict ionization- induced symmetry breaking in the FA dimer ion ground state that results in ultrafast

proton transfer concerted with opening of the dimer ring structure. Moreover, our coincidence analysis combined with theoretical simulations revealed the ultraslow delayed dissociation of dimer cation to FAH^+ and $FA - H$ product on the s timescale. Two- and three-body Coulomb explosion channels of FA dimer cation will also be discussed.

[1] E. Livshits et al., Symmetry-breaking dynamics of a photoionized carbon dioxide dimer, Nat Commun 15, 6322 (2024).

#B57: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Autodetachment and autofragmentation in anionic species

Sergio Sánchez Pinel¹; Jesús González-Vázquez¹; Alicia Palacios¹; Michael Gatchell²; MingChao Ji²; Stefan Rosén²; Henrik Cederquist²; Henning Schmidt²; Henning Zettergren²; Fernando Martín¹

¹ Departamento de Química, Universidad Autónoma de Madrid

² Department of Physics, Stockholm University, 106 91 Stockholm, Sweden

The XCHEM method[1] allows the study of ultrafast processes in anions. At the core of the XCHEM method lies the Gaussian-B-spline basis (GABS)[2], used to represent bound and continuum states. It has been successfully applied to cations, such as neon[2], nitrogen[3] and carbon monoxide[4]. This formalism has started recently to be applied to anions, using nitrogen N_2^- as a benchmark to assess the validity of this method.

C_2^- is a rather stable molecule, with lower energy than that of the C_2 , but it has been shown that in excited vibronic molecules, the system goes through either a process of autodetachment, resulting in $C_2 + e^-$, and fragmentation, resulting in $C^- + C$ [5,6].

The anion relevant states for these processes are the first 3 doublet states ($X^2\Sigma_g^+$, $A^2\Pi_u$ and $B^2\Sigma_u^+$) and the first quadruplet ($a^4\Sigma_u^+$), higher in energy. The relevant states for the neutral molecule in this work are the first two: $X^1\Sigma_g^+$ and $a^3\Pi_u$. A thorough study of these channels have been done, calculating the relevant contributions for a kinetic calculation, taking into account the radiative processes that can occur at the same time. XCHEM has never been used in such extensive work with an anionic species, and in this communication we present the some results from the ongoing study.

[1] C. Marante et al., J. Chem. Theory Comput. 13, 499-514 (2017).

[2] C. Marante et al., Phys. Rev. A. 9, 012506 (2014).

[3] M. Klinker et al., J. Phys. Chem. Lett. 9, 756 (2018).

[4] V. J. Borràs et al., J. Chem. Theory Comput. 17, 6330 (2021).

[5] V. C. Schmidt et al., Phys. Rev. A. 110, 042828 (2024).

[6] V. C. Schmidt et al., Phys. Rev. Lett. 133, 183001 (2024)

#B58: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

All-optical coherent control of chiral electronic transitions for highly enantioselective photochemistry

Andrés Ordóñez¹; David Ayuso²; Patricia Vindel-Zandbergen³

¹ Imperial College London / Freie Universität Berlin

² Imperial College London, Department of Chemistry, UK

³ New York University, Department of Chemistry, USA

Circularly polarized light (CPL) induces different populations in left- and right-handed versions of randomly oriented chiral molecules. Such differences lead to differences in the product yields of photochemical reactions. Thus, CPL triggers all-optical enantioselective photochemistry. But the difference is usually below 0.1%, rendering CPL impractical for photochemical applications. Therefore, photochemistry still invariably relies on chemical (instead of all-optical) methods to control enantioselectivity. A practical all-optical alternative would allow unprecedented temporal and spatial control over the enantioselectivity of photochemical reactions. Beyond applications like enantiomeric enrichment, such control would also enable new technologies, like enantiomeric switches [2], which are currently hindered by CPL's low selectivity.

Here we introduce two schemes (see Fig. [1]) to enantioselectively control the excited state population of electronic states in chiral molecules. Our proposal [3] can be realized using readily available fs technology [4], requires neither all-resonant transitions nor long electronic coherence times, and yields enantioselectivities close to 30%. Our findings are supported by analytical theory revealing the role of light's polarization in both schemes, and by ab-initio simulations.

In the 1- vs 2-photon scheme, we find that the enantioselectivity oscillates on the scale of the fundamental wavelength. Thus, maintaining enantioselectivity requires constraining the interaction region accordingly, e.g. using appropriately oriented thin flat liquid microjets. We find that the oscillation of the enantioselectivity across the interaction region can be avoided by using the 2- vs 3-photon scheme in Fig. 1b. Including liquid water dispersion yields oscillations on the scale of 50 μm , which can be easily addressed.

Fig. [1]: [2] B L Feringa, *Angew. Chem. Int. Ed.* 56, 11060 (2017)

[3] A Ordóñez et al., arXiv 2309.02392 (2023)

[4] C Burger et al., *Opt. Express* 25, 31130 (2017)

#B59: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Ultra-fast nonlinear optical response of chiral molecules with a focus on conformer sensitivity

Elena Aethra Christou¹; Felipe Morales²; David Ayuso³; Olga Smirnova²

¹ Max Born Institute for Nonlinear Optics and Short Pulse Spectroscopy

² Max-Born-Institute for Nonlinear Optics and Short Pulse Spectroscopy, Berlin, 12489, Germany

³ Department of Chemistry, Molecular Sciences Research Hub, Imperial College London, W12 0BZ London, UK

Chirality is a fundamental geometric property, present from molecular to macroscopic scales. Traditional chiroptical methods rely on weak

magnetic interactions, limiting their efficiency. We aim to develop chiral recognition methods based solely on electric-dipole interactions, offering enhanced enantiosensitivity [1].

We investigate the carrier-envelope phase (CEP) dependence of enantio-sensitive observables within the electric dipole approximation by numerically analyzing the nonlinear response of randomly oriented chiral molecules in the gas phase. Using time-dependent density functional theory (TDDFT), we model their interaction with few-cycle, tightly focused, CEP-controlled linearly polarized laser pulses. Tight focusing induces a longitudinal field component, creating a forward-elliptically polarized field [2]. This drives a chiral response perpendicular to the polarization plane, leading to the emission of even-order chiral harmonics in addition to the odd-order achiral harmonics. Their CEP-dependent interference results in enantiosensitive nonlinear optical rotation [2]. Here we explore the sensitivity of the CEP-dependent signal to chiral molecular conformations and the uniqueness of the CEP molecular markers.

We focus on the chiral dynamics of essential amino acids, using serine as a prototypical case. We analyze its three dominant conformers in the gas phase, with relative populations of 43.7%, 18.8%, and 14.8% [3]. By placing a polarizer before the detector, one can convert enantio-sensitive polarization properties into an enantio-sensitive intensity distribution, which can be considered as chiral "QR codes" mapping the chiral dichroism of emitted harmonics as a function of the CEP of the incident light. We show that chiral dichroism (CD) vs. CEP has different patterns for different conformers (note that for the same harmonic order, the CD maximizes at different CEP values in serine I and serine II), reflecting different molecular phase accumulation due to ultrafast electron dynamics in two conformers and making chiral QR codes suitable for molecular fingerprinting.

We gratefully acknowledge ERC-2021-AdG project ULISSES, grant agreement No. 101054696.

References:

[1] D. Ayuso *et al.*, *PCCP* 24, 26962 (2022). DOI: [10.1039/D2CP01009G](https://doi.org/10.1039/D2CP01009G)

[2] D. Ayuso *et al.*, *Optica* 8, 1243 (2021). DOI: [10.1364/NLO.2021.NW2A.2](https://doi.org/10.1364/NLO.2021.NW2A.2)

[3] K. He and W. D. Allen, *J. Chem. Theory Comput.* 12, 3571 (2016). DOI: [10.1021/acs.jctc.6b00314](https://doi.org/10.1021/acs.jctc.6b00314)

#B60: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Modelling sequential ionisation within time-dependent R-Matrix Theory

Holly Lavery; Andrew Brown; Hugo van der Hart

Queen's University Belfast

We present a new approach to model sequential ionization processes, employing a series of R-matrix with time-dependence (RMT) calculations to model the behaviour of the residual ion stages, and a density matrix to describe the coherences between the residual ion states. This combination allows us to describe correlated dynamics through multiple ionization stages.

RMT is a technique that can study the dynamics present in laser-driven, multielectron system on ultrafast timescales [1]. RMT partitions the system into two distinct regions. In the 'inner' region (close to the nucleus), the correlation between electrons is described fully. In the 'outer' region, electron exchange is neglected, and an ionized electron moves under the influence of the laser and the long-range potential of the ion.

Density matrix theory has been applied to understand the attosecond-scale dynamics (see [2] for an example studying correlations between photoelectrons in sequential photoionization). The density matrix can summarise the ionic quantum state left after ionization. The population of the residual ion states is contained in the diagonal elements,

while the off-diagonal elements contain the correlation coefficients between these states.

As a demonstration, we model pump-probe ionisation of Ne^+ to Ne^{3+} using an XFEL with photon energies of 95 eV [3]. We start with Ne^+ in its $2p^o$ ground state with either $m = 0$ or $m = 1$. An initial XUV photon ionizes Ne^+ to Ne^{2+} . After a time delay (up to 1.2 fs), a second XUV pulse photoionises Ne^{2+} to Ne^{3+} . The main observable of interest is the momentum-resolved angular distribution of the photoelectrons. Separate angular distributions are obtained for each residual ion state, including orbital and spin magnetic quantum numbers.

The angular distribution of the outgoing electron is affected by changes in delay time. For a delay time of 0.39 fs, the distribution is more aligned along the polarization axis compared to a delay time of 0.94 fs. This change is caused by the coherent superposition of the Ne^{2+} ion after ionisation by the pump pulse. This superposition is seen for the $m = 0$ levels of the $1S$ and $1D$ states, as these two states are built from the same independent electron basis states.

[1] A. Brown *et al.*, *Comput. Phys. Commun.*, 250 107062 (2020)

[2] L.A.A Nikolopoulos, *Phys. Rev. Lett.* 111 093001 (2013)

[3] W. Decking *et al.*, *Nat. Photonics*, 14 391-397 (2020)

#B61: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Excited-State Dynamics of Pyrazine and the Role of Electronic Coherences

Luke Moore¹; Micheal J. Bearpark²; Graham Worth³; Mike A. Robb²

¹ Imperial College London : Department of Chemistry

² Imperial College London

³ University College London

Recent advances in attoscience have revealed that electron cloud dynamics, driven by superpositions of electronic states, can influence nuclear motion and, in turn, chemical reactivity [1]. In excited-state processes, conical intersections (CIs) play a central role and are both sensitive to and capable of generating electronic coherences—superpositions where overlapping electronic states interfere within the same spatial region.

Using pyrazine as a model system, we investigate the excited state decay mechanism from the S_2 state, which occurs by passing through the S_2 - S_1 CI, through a combination of electronic structure calculations and dynamics simulations (semi-classical Second-Order [2] and fully quantum mechanical Quantum Ehrenfest [3] methods paired with CASSCF). Our results support the historically accepted view that only optically bright states contribute significantly to the decay. However, we also explore the influence of electronic coherences in this process.

Consistent with symmetry-based theoretical predictions [4], we find that coherences do not form between states of different Abelian point group symmetry at the Franck-Condon region. Crucially, we show that this restriction can be bypassed: even a slight initial mixture of states (e.g., a 99:1 population ratio) breaks the symmetry constraint and allows coherence formation—offering a theoretical explanation for recent experimental observations [5].

References

[1] I. C. D. Merritt *et al.*, *J. Phys. Chem. Lett.*, 2021, **12**, 8404–8415

[2] M. Vacher *et al.*, *Theor. Chem. Acc.*, 2014, **133**, 1505

[3] A. J. Jenkins *et al.*, *J. Chem. Phys.*, 2018, **149**, 094108

[4] S. P. Neville *et al.*, *J. Phys. B: At. Mol. Opt. Phys.*, 2022, **55**, 044004

[5] Y. P. Chang *et al.*, *Nat. Phys.*, 2025, **21**, 137–145

#B62: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Electronic coherences in molecules with XFAIMS

Celso Manuel González-Collado¹; Amiel Paz²; Todd J. Martínez²; Fernando Martín³; Alicia Palacios⁴

¹ Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain

² Department of Chemistry, Stanford University, Stanford, California 94305, United States. Stanford PULSE Institute, SLAC National Accelerator Laboratory, Menlo Park, California 94025, United States

³ Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain. Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA-Nanociencia), Cantoblanco, 28049 Madrid, Spain. Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain

⁴ Departamento de Química, Módulo 13, Universidad Autónoma de Madrid, 28049 Madrid, Spain. Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, 28049 Madrid, Spain. Institute for Advanced Research in Chemical Sciences (IAdChem), Universidad Autónoma de Madrid, 28049 Madrid, Spain

To access the natural timescale of electronic motion in molecules, attosecond resolution is needed. But triggering such ultrafast dynamics in excited molecules requires UV/Vis ultrashort pulses, of just a few femtoseconds. These pulses, that are becoming increasingly available in recent years [1], have a broad energy bandwidth, which creates a superposition of electronic excited states, followed by coupled electron-nuclear non-adiabatic dynamics that can affect the initial electronic coherences. The development of an appropriate framework to model such dynamics is crucial to correctly interpret hypothetical pump probe experiments capable of monitoring those electronic coherences in real time. Because of that, we are currently working on a modified version of Ab Initio Multiple Spawning (AIMS) methodology [2], that propagates the dynamics through frozen gaussian functions following classical trajectories. This choice is justified because AIMS has a much lower computational cost than fully quantum methods (such as multi-configuration time-dependent Hartree), but it is still able to accurately describe electronic coherences from the very beginning with some improvements of the standard program [3], in contrast to more classical methods such as Trajectory Surface Hopping. In this work, we implement for the first time the AIMS methodology to model electronic coherences between multiple excited states in multielectronic diatomic and small polyatomic molecules, where quantum approaches are also at hand. It is worth highlighting that we took advantage of the software TeraChem to carry out the electronic structure calculations due to its capability to run on GPUs, which are considerably faster than the usual CPUs [4]. We also analyze the sensibility of these coherences to different parameters of the simulation, such as the initial basis set of coupled gaussian functions, the spawning threshold, the order of approximation of Hamiltonian matrix elements and the explicit inclusion of the laser pulse (XFAIMS [5]).

[1] M. Reduzzi *et al.*, *Optics Express* 31, 16 (2023)

[2] B. Curchod and T. Martínez, *Chem. Rev.* 118, 7 (2018)

[3] B. Mignolet and B. Curchod, *J. Chem. Phys.* 148, 134110 (2018)

[4] I. Ufimtsev and T. Martínez, *J. Chem. Theory Comput.* 5, 10 (2009)

[5] B. Mignolet, B. Curchod and T. Martínez, *J. Chem. Phys.* 145, 19 (2016)

TOMATTO project has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme (grant agreement No 951224).

#B63: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Methods for analysing photoelectron momentum distributions from attosecond light pulses

Emilia Kjærdsdam Telléus; Praveen Kumar Maroju; Daniel Díaz Rivas; Nedjma Ouahioune; Jan Marcus Dahlström; Anne L'Huillier; Cord L. Arnold; Mathieu Gisselbrecht

Department of Physics, Lund University, Lund, Sweden

The three-dimensional momentum distribution of photoelectrons is determined by conservation laws embodied in the selection rules and depends on the state of the ionising light fields. The process of high harmonic generation, allows for the creation of light pulses of attosecond duration [1, 2], and the measurement of photoelectron momentum distributions following from the interaction with these, is an important tool for gaining insight in the ultrafast dynamics of light-matter interaction. Recent developments and proposals in the tailoring of the polarisation and spatial properties of such attosecond pulses [3, 4, 5, 6] opens new possibilities for using light fields of exotic configurations in photoionisation experiments, further motivating the improvement of methods for understanding and analysing complex photoelectron momentum distributions. Here, we present a method, which consists both of theoretical simulations of three-dimensional photoelectron distributions, and of an algorithm for decomposing an unknown distribution in a coherent sum of spherical harmonics, with the aim of determining the angular momentum quantum numbers. The theoretical simulation is based on the strong field approximation, and takes as input light fields of a specified configuration, encompassing the number of pulses, their polarization, carrier-to-envelope phase, and the delay between them. This enables investigations of the effect of different features of the light field on the photoelectrons. We intend to demonstrate that this double-sided mathematical tool is robust, within limitations, in the characterisation of photoelectron momentum distributions.

References

- [1] P B Corkum, *Phys. Rev. Lett.* 71, 1994 (1993)
- [2] P Antoine et al., *Phys. Rev. Lett.*, 77 1234 (1996)
- [3] J M N Djiokap et al., *Phys. Rev. Lett.*, 115, 113004 (2015)
- [4] Rego, L. et al., *Science*, 364, 1253 (2019)
- [5] Ayuso, D. et al., *Nat. Photonics*, 13, 866 (2019)
- [6] Habibović, D. et al., *Nat. Rev. Phys.*, 6, 663 (2024)

#B64: Fundamental physics, precision measurements, atom interferometry and atomic clocks

New magic wavelength for Sr clock transition

Xin Yuan Ma¹; Swarup Das²; Chang Chi Kwong²; David Wilkowski²

¹ Center for quantum technologies, National university of singapore

² Nanyang Quantum Hub, School of Physical and Mathematical Sciences, Nanyang Technological University

Optical lattice operating at the magic wavelength induces identical AC-Stark shifts on two internal states of trapped atoms, permitting a coherent control of the transition. The characteristics is vital for quantum applications based on cooled neutral atoms, including quantum computing, atom clock and precision metrology.

We discovered a new magic wavelength at 476.823545(55) nm for ⁸⁸Sr clock transition between the ground ¹S₀ and the metastable ³P₀ states. When used as Bragg diffraction pulses in the clock atom interferometry, the new magic wavelength provides a larger momentum kick to

the atoms compared with the usual magic wavelength at 813.4 nm. This facilitates a greater separation between the two momentum states, thereby enhancing the sensitivity of atom interferometer. The optical lattice at around 477 nm also has a smaller lattice constant, making it potentially useful for quantum simulation and studies of cooperative effects. Additionally, the result also provides a valuable reference for determining electric dipole matrix elements of nearby atomic transitions.

#B65: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Squeezing-enhanced accurate differential sensing under large phase noise

Marco Malitesta¹; Robin Corgier²; Leonid A. Sidorenkov²; Franck Pereira Dos Santos²; Gabriele Rosi³; Guglielmo Maria Tino⁴; Augusto Smerzi⁵; Leonardo Salvi⁶; Luca Pezzè⁵

¹ Istituto Nazionale di Ottica, Consiglio Nazionale delle Ricerche (INO-CNR), Department of Physics and Astronomy, Università di Firenze

² LTE, Observatoire de Paris, Université PSL, Sorbonne Université, Université Lille, LNE, CNRS

³ Department of Physics and Astronomy, Università di Firenze, Istituto Nazionale di Fisica Nucleare (INFN)

⁴ Istituto Nazionale di Ottica, Consiglio Nazionale delle Ricerche (INO-CNR), Department of Physics and Astronomy, Università di Firenze, Istituto Nazionale di Fisica Nucleare (INFN), European Laboratory for Nonlinear Spectroscopy (LENS)

⁵ Istituto Nazionale di Ottica, Consiglio Nazionale delle Ricerche (INO-CNR), European Laboratory for Nonlinear Spectroscopy (LENS), QSTAR

⁶ Department of Physics and Astronomy, Università di Firenze, Istituto Nazionale di Fisica Nucleare (INFN), European Laboratory for Nonlinear Spectroscopy (LENS)

Atom interferometers are reaching sensitivities fundamentally constrained by quantum fluctuations [1]. A main challenge is to integrate entanglement into quantum sensing protocols to enhance precision while ensuring robustness against noise and systematics [2-4]. Here, we theoretically investigate differential phase measurements with two atom interferometers using spin-squeezed states [5], accounting for common-mode phase noise spanning the full 2π range. We estimate the differential signal using model-free ellipse fitting [6], a robust method requiring no device calibration and resilient to additional noise sources. Our results show that spin-squeezing enables sensitivities below the standard quantum limit (SQL). Specifically, we identify optimal squeezed states that minimize the differential phase uncertainty, scaling as $N^{-2/3}$, thus overcoming the SQL, while eliminating the bias inherent in ellipse fitting methods. We benchmark our protocol against the Cramér-Rao bound and compare it with hybrid methods that incorporate auxiliary classical sensors. Our findings provide a pathway to robust and high-precision atom interferometry, in realistic noisy environments and using readily available states and estimation methods.

[1] L. Pezzè, A. Smerzi, M. K. Oberthaler, R. Schmied, and P. Treutlein, *Quantum metrology with nonclassical states of atomic ensembles*, *Rev. Mod. Phys.* **90**, 035005 (2018)

[2] A. André, A. S. Sørensen, and M. D. Lukin, *Stability of Atomic Clocks Based on Entangled Atoms*, *Phys. Rev. Lett.* **92**, 230801 (2004).

[3] B. Braverman, A. Kawasaki, and V. Vuletić, *Impact of non-unitary spin squeezing on atomic clock performance*, *New. J. Phys.* **20**, 103019 (2018)

[4] L. Pezzè and A. Smerzi, *Heisenberg-Limited Noisy Atomic Clock Using a Hybrid Coherent and*

Squeezed State Protocol, *Phys. Rev. Lett.* **125**, 210503 (2020).

[5] M. Kitagawa and M. Ueda, Squeezed spin states, *Phys. Rev. A* **47**, 5138 (1993)

[6] G. T. Foster, J. B. Fixler, J. M. McGuirk, and M. A. Kasevich, Method of phase extraction between coupled atom interferometers using ellipse-specific fitting, *Opt. Lett.* **27**, 951 (2002).

#B66: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Hydrogen atom diffraction through free-standing single-layer graphene

Pierre GUICHARD¹; Arnaud Dochain²; Raphaël Marion³; Pauline de Crombrughe de Picquendaele²; Nicolas Lejeune⁴; Benoît Hackens²; Paul-Antoine Hervieux¹; Xavier Urbain²

¹ Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg

² Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain

³ Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, Royal Observatory of Belgium (ROB-ORB)

⁴ Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, EPHEC

Hydrogen atom diffraction through free-standing single-layer graphene

Pierre Guichard,¹ Arnaud Dochain,² Raphaël Marion,^{2,3} Pauline de Crombrughe de Picquendaele,² Nicolas Lejeune,^{2,4} Benoît Hackens,² Paul-Antoine Hervieux,¹ and Xavier Urbain²

¹ Université de Strasbourg, CNRS, Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504, 67000 Strasbourg, France

² Institute of Condensed Matter and Nanosciences, Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium

³ Royal Observatory of Belgium (ROB-ORB), B-1180 Brussels, Belgium

⁴ EPHEC, B-1348 Louvain-la-Neuve, Belgium

We report the observation of fast atom diffraction through single-layer graphene. High resolution images have been recorded with hydrogen atoms at kinetic energies ranging from 150 eV to 1200 eV, following the experimental protocol suggested by Brand et al. [1]. The commercial suspended graphene samples were characterized using micro-Raman spectroscopy, prior to and after beam exposure for the quantification of defects. When placed on the beam path in ultra-high vacuum, the samples were subjected to high temperature to induce thermal desorption of contaminants. Monocrystalline domains within the illuminated area produced characteristic hexagonal diffraction patterns. A negligible energy loss was recorded by time-of-flight tagging of individual atom detection events, making such an experimental approach suitable for matter-wave interferometry.

Density functional theory calculations with pseudopotentials [2] have been performed to determine the H-graphene interaction potential over the whole unit cell. The total energy of the system was calculated as a function of the position of the hydrogen atom relative to the graphene surface. The energies of the isolated graphene sheet and the hydrogen atom were then subtracted from the total energy of the system. Nice agreement with the calculations of Ehemann et al [3] is found, who used the Self-Consistent Charge-Density Functional Tight Binding method. In particular, our calculations confirm the presence of a long-range potential well reminiscent of the C-H bond. In order to simulate diffraction images, we generate a phase mask by integrating the three-dimensional potential along the coordinate normal to the graphene plane and performing an eikonal treatment of the scattering events.

[1] C. Brand, M. Debiossac, T. Susi, F. Aguilon, J. Kotakoski, P. Roncin, and M. Arndt, *New Journal of Physics* **21**, 033004 (2019)

[2] P. Giannozzi, S. Baroni, N. Bonini, et al., *Journal of Physics: Condensed Matter* **21**, 395502 (2009)

[3] R. C. Ehemann, P. S. Krstić, J. Dadras, P. R. C. Kent, and J. Jakowski, *Nanoscale Research Letters* **7**:198 (2012)

#B67: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Cold Rydberg Strontium Atoms for the Thermometry of Optical Lattice Clocks

Hugo Tortel¹; Jérôme Lodewyck²; Patrick Cheinet³

¹ Laboratoire Aimé Cotton, Paris-Saclay University and Laboratoire Temps Espace, Paris Observatory

² Laboratoire Temps Espace, Paris Observatory

³ Laboratoire Aimé Cotton, Paris-Saclay University

The relentless pursuit of higher precision in optical lattice clocks (OLC) demands ever more refined methods to mitigate environmental perturbations, with blackbody radiation (BBR) induced frequency shifts standing as a major challenge. State-of-the-art OLCs address this effect by either operating in a cryogenic environment to reduce the BBR [1], by employing comprehensive temperature monitoring and compensation techniques in room-temperature setups [2] or by shielding the in-vacuum radiation inhomogeneities [3].

Atoms excited to Rydberg states have been proposed, due to their enhanced sensitivity to BBR [4], as excellent candidates for in-situ and calibration-free measurements of the BBR spectrum experienced by atoms in OLCs [5]. This approach relies on measuring the BBR-induced energy shifts of Rydberg states but is challenging due to the absence of a well-defined reference state. To overcome this limitation, a method based on BBR-induced state transfers has been proposed [6]. A theoretical model, developed alongside new experimental results using alkali Rubidium atoms [7], demonstrates promising initial results and a first validation of this technique.

Until now, proposed methods and models have relied on Rydberg physics in alkali atoms, whereas OLCs are based on alkaline-earth atoms. Divalent atoms introduce new challenges in the theoretical treatment of Rydberg physics, which is already complex for alkali atoms. However, the presence of two valence electrons in alkaline-earth Rydberg atoms unlocks a range of new behaviors and phenomena [8]. We will present a new theoretical protocol, specific to divalent Rydberg atoms, harnessing their unique effects. We will then analyze its merit compared to the existing protocols. An experiment is currently being built to demonstrate the feasibility of this method.

[1] I. Ushijima et al. *Nature Photonics* **9**, 185–189, (2015)

[2] Y. Foucault et al. *Joint Conference of the European Frequency and Time Forum and IEEE International Frequency Control Symposium (EFTF/IFCS)*, (2021)

[3] K. Beloy et al. *Phys. Rev. Lett.* **113**, 260801, (2014)

[4] T.F. Gallagher. *Cambridge Monographs on Atomic, Molecular, and Chemical Physics*, (1994)

[5] V.D. Ovsiannikov et al. *Phys. Rev. Lett.* **107**, 093003, (2011)

[6] E.B. Norrgard et al. *New J. Phys.* **23**, 033037, (2021)

[7] N. Schlossberger et al. *Phys. Rev. Research* **7**, L012020, (2025)

[8] K.L. Pham et al. *PRX Quantum* **3**, 020327, (2022)

#B68: Fundamental physics, precision measurements, atom interferometry and atomic clocks

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

Shirley Zheng; Rhys Jenkins; Freddie Collings; Elise Wursten; Michael Ziemba; Ferruccio Castellini; Jongseok Lim; Ben Sauer; Michael Tarbutt

Imperial College London

The standard model predicts a value for the electron's electric dipole moment (eEDM, d_e), $d_e \sim 10^{-35}$ e cm [1], far smaller than what is predicted by theories beyond the standard model, typically $d_e \approx 10^{-31} - 10^{-24}$ e cm. To date, the current experimental upper limit is set at $d_e < 4.1 \times 10^{-30}$ e cm [2]. Further improvements in experimental precision are likely to discover new physics or rule out much 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 collimated ultracold YbF molecules produced by a cryogenic buffer gas source and then laser cooled to 100 uK in the two transverse axes [3]. Such cooling increases beam brightness and spin-precession time, leading to a projected statistical uncertainty below 10^{-30} e cm [4]. However, magnetic field noise can severely limit the precision of our phase sensitive measurement of d_e . To overcome this source of noise, we have developed and characterised a novel spin precession region, including ceramic electric field plates, a glass vacuum chamber, magnetometry, and a four-layer magnetic shield with a shielding factor $> 10^5$ [5]. We prepare the eEDM-sensitive state using stimulated Raman adiabatic passage and detect the molecules with near unit efficiency. We are currently working to reach the shot noise limit of statistical sensitivity.

References

- [1] Ema, Y. et al, 2022, Phys. Rev. Lett., 129, 231801
- [2] Roussy T. et al, 2023, Science, 381, 46-50
- [3] Alauze X. et al, 2021, Quantum Sci. Technol., 6, 044005
- [4] Fitch N. J. et al, 2021, Quantum Sci. Technol., 6, 014006
- [5] Collings F. et al, 2025, arXiv:2503.21725v1

#B69: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Optical Frequency Division for Ultra-Stable Microwave Generation and Remote Clock Referencing

Benjamin Pointard; Michel Abgrall; Michel Lours; Paul-Eric Pottie; Rodolphe Le Targat

LNE-OP, Laboratoire Temps Espace, Observatoire de Paris PSL

The generation of ultra-stable microwave signals with low phase noise is a fundamental requirement for high-precision atomic clocks. In particular, state-of-the-art microwave fountains, such as those based on cesium (Cs) and rubidium (Rb) atoms, operate at the quantum projection noise (QPN) limit, where the stability of the interrogation signal plays a critical role. At LNE-OP, we have developed an optically derived microwave source that leverages the superior stability of optical oscillators. This technique relies on the frequency division of a 1542 nm ultrastable laser using an optical frequency comb (OFC), enabling the generation of a spectrally pure 11.98 GHz signal. This microwave

signal is essential for probing atomic transitions in Cs and Rb fountains, maintaining high short-term stability.

To achieve long-term stability, the optical reference is initially frequency-locked to a hydrogen maser, ensuring proper tracking of long-term drifts. An additional phase-lock is implemented to eliminate residual long-term offsets, maintaining strict phase coherence necessary for precision timekeeping. The laser, originally stabilized to an ultrastable cavity, exhibits a frequency stability of 5×10^{-16} at 1 s. The optical frequency comb, based on an erbium-doped fiber laser, ensures precise frequency division from the optical to the microwave domain. A digital phase-lock system further compensates for residual frequency drifts, maintaining an output stability at the 10^{-15} level.

This new system effectively replaces the previous cryogenic sapphire oscillator (CSO), which, due to helium shortages, is now operational only at critical times. Our approach offers a viable and sustainable alternative while maintaining comparable or superior performance across key stability metrics. Furthermore, it provides LNE-OP with a complete microwave architecture to fully exploit the PHARAO-ACES space clock ensemble (launched in April 2025). The full implementation relies on a stabilized fiber-optic link that distributes the 1542 nm signal with minimal added phase noise.

Beyond the controlled laboratory environment, we extend this technology towards field-deployable optical clocks, where maintaining an accurate RF reference under remote conditions becomes critical. These transportable systems require a robust local RF reference to enable precise frequency measurements outside laboratory infrastructure. To address this challenge, we demonstrate the bootstrapping of an OFC to an accurate 1542 nm reference signal disseminated via the REFIMEVE+ fiber network. This network delivers an ultrastable optical carrier across laboratories, and our approach ensures the local generation of low-noise RF signals at 10 MHz and 1 GHz in remote environments. By leveraging this infrastructure, we enable high-precision frequency synthesis, facilitate remote clock comparisons between metrology institutes, and strengthen the robustness of optical clock networks.

In addition to fiber-based dissemination, we investigate an alternative approach that eliminates the need for external optical or RF references. This method involves directly bootstrapping the frequency comb to an optical clock laser, a strategy particularly suited for autonomous or mobile clock applications. The clock laser inherently carries the high accuracy and stability of the atomic transition it probes. Through frequency division by the OFC, we can extract a local RF reference at 10 MHz or 1 GHz, essential for clock operation and electronic synchronization. This technique ensures that optical clocks can operate independently in environments where fiber-based references are unavailable, thereby expanding the reach of high-precision timekeeping beyond traditional infrastructure.

Preliminary experimental results validate the feasibility of these approaches, demonstrating excellent stability and phase noise performance both in laboratory settings and in remote configurations. Our findings indicate that optically derived microwaves can serve as robust replacements for traditional RF sources, opening new pathways for advanced time and frequency metrology. Future work will focus on optimizing phase noise characteristics, integrating these systems into international clock comparison networks, and further developing the standalone optical clock bootstrapping technique for real-world field applications.

#B70: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Molecular spectroscopy in the THz range under sub-Doppler regime

Andjela Zarin¹; Luan Juppert¹; Olivier Pirali²

¹ ISMO/U. Paris Saclay

² ISMO CNRS/U.Paris-Saclay

Terahertz (THz, 0.1-10 THz) precision spectroscopy of various molecular species is essential for several applications such as astrophysics and planetary atmosphere sensing, molecular physics, and tests of fundamental physics, yet it remains technically challenging. Such measurements require on one side the development of a dedicated spectrometer allowing for broadband measurements at ultra-high resolution (and for which the frequency axis is referenced to SI frequency standards) and on the other side to develop methodologies to probe the molecular transitions under sub-Doppler regime in order to resolve the finest intramolecular couplings. Both considerations are challenging in the THz range. In the present poster, we will present our current efforts to obtain THz absorption spectra of various molecules under sub-Doppler regime using a THz frequency multiplication chain. The frequency axis of our measurements is referenced to SI standard thanks to the recent reception of both RF and optical frequency references provided by the SYRTE laboratory and disseminated by the REFIMEVE+ network.

We tested two different approaches to record sub-Doppler spectra for non-reactive molecular species up to 1.5THz: double resonance (Mid-IR pump and THz probe) and saturated absorption experiments. These two techniques were used to measure the pure rotational transitions of ammonia (NH₃) and methane (CH₄). We will present the experimental set-up we developed and the spectroscopy results obtained for both molecules. In particular the observation of the finest coupling in NH₃ (coupling of the H spins with the rotation angular momentum) allows us to determine the molecular structure in the ground and the first vibrationally excited state.

#B71: Fundamental physics, precision measurements, atom interferometry and atomic clocks

The ground state hyperfine splitting in muonic hydrogen experiment (HyperMu) at PSI

Ahmed Ouf¹; CREMA collaboration²

¹ Johannes Gutenberg Universität mainz

² Paul Scherrer Institute

The HyperMu experiment at PSI aims at the first measurement of the ground state hyperfine splitting in muonic hydrogen (μp) with 1 ppm precision using pulsed laser spectroscopy. This accuracy allows for a precise extraction of the proton structure contributions, including the Zemach radius and the proton polarizability.

To measure the ground state hyperfine splitting in μp , we are developing a unique pulsed laser system designed to deliver 4 mJ pulses at a wavelength of 6.8 μm , randomly triggered upon muon detection. We report on the latest laser development within the experiment, the several developments of the detection system that was carried out and the optimization of the experimental parameters to obtain a successful resonance signal.

#B72: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Chip-scale Rydberg Quantum Electrometry

Avital Giat; Kfir Levi; Liron Stern; Ori Nefesh

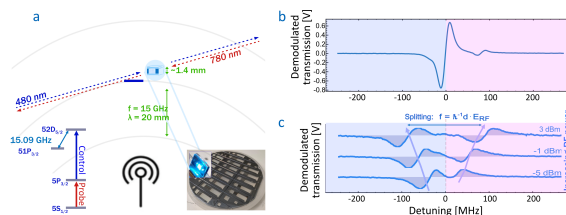
The Hebrew University of Jerusalem

In the past decade, Rydberg atoms have emerged as promising and valuable tools for a myriad of quantum applications, and particularly quantum sensors. The exaggerated properties of Rydberg atoms make them highly sensitive to electric fields spanning from DC to THz frequencies, which makes them an appealing tool for sensitive, accurate, and simple sensors. This field is of tremendous interest to a wide range of industries, particularly electric field sensing. Indeed, much work has been done showcasing sensitive, accurate and cost-effective atomic Rydberg sensors. While numerous demonstrations have realized such sensors using centimeter-scale vapor cells [1,2], efforts to miniaturize Rydberg-based field sensors to millimeter footprints remain scarce.

Leveraging advances in wafer-scale microfabrication—which have already transformed chip-scale atomic clocks and magnetometers [3]—we present an all-optical, sub-wavelength radio-frequency (RF) sensor based on micromachined rubidium vapor cells with millimeter-scale dimensions (Fig. b). We systematically investigate how proximity-induced electrostatic fields influence the Rydberg lineshape by varying cell temperature, laser power, atomic density, and beam position. Rydberg excitation is achieved via electromagnetically induced transparency (EIT) using counter-propagating 780 nm (probe) and 480 nm (pump) lasers to access the $52D_{5/2}$ state (Fig. a). Figure b shows a representative EIT lineshape obtained in a 1.4 mm cell. We then apply an RF field at 15.09 GHz ($52D_{5/2} \rightarrow 51P_{3/2}$ transition) via an antenna ≈ 15 cm from the cell, inducing Autler–Townes splitting that enables direct RF amplitude measurements (Fig. c).

We observe clear Autler–Townes doublets whose splitting scales with the applied RF amplitude. Beyond the expected monotonic increase in linewidth and contrast, we report lineshape shifts, broadening, and asymmetry as temperature and pump power increase—signatures of DC Stark shifts arising from static fields. We attribute these fields to photoionization-induced charges on the cell walls and thermally activated surface charging. Spatially resolved measurements further reveal a nonuniform electrostatic-field profile within the cell.

Finally, the RF resonance exhibits an ≈ 20 MHz redshift relative to its calculated value. By incorporating DC-Stark shifts and inhomogeneous broadening into our EIT simulations, we estimate a ~ 0.2 V/cm DC field. This modeling informs optimized spectroscopic conditions, substantially improving signal-to-noise performance (Fig. c).



00

In summary, we demonstrate Rydberg-based electrometry in millimeter-scale, wafer-fabricated vapor cells that enable broadband, ultra-sensitive, non-invasive sub-wavelength RF field detection [4]. We characterize the EIT lineshape under varying electrostatic conditions at the cell windows, identify how surface charging and temperature-induced effects impact sensor performance, and introduce mitigation strategies to preserve spectroscopic fidelity. These results chart a clear pathway toward fully integrated, chip-scale Rydberg electric-field sensors with sub-wavelength resolution.

[1] Simons, Matthew T., et al. “A Rydberg atom-based mixer: Measuring the phase of a radio frequency wave.” *Applied Physics Letters*

114.11 .(2019)

[2] A. Duspayev, R. Cardman, D. A. Anderson, and G. Raithel, “High-angular-momentum rydberg states in a room-temperature vapor cell for dc electric-field sensing,” *Phys. Rev. Res.* **6**, 023138 (2024).

[3] Kitching, John. “Chip-scale atomic devices.” *Applied Physics Reviews* **5.3** .(2018)

[4] Giat, Avital, et al. “Subwavelength micromachined vapor-cell based Rydberg sensing.” *arXiv preprint arXiv:2504.09559* (2025).

#B73: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Stringent Tests of Theory via High Precision Measurements with Single Ions in the ALPHATRAP Experiment

Fabian Heiße¹; Matthew Bohman¹; Charlotte M. König¹; Ivan Kortunov²; Jonathan Morgner¹; Victor Vogt²; Klaus Blaum¹; Stephan Schiller²; Sven Sturm¹

¹ Max-Planck-Institut für Kernphysik

² Heinrich Heine University Düsseldorf

The Standard Model of particle physics very successfully describes a broad range of physical phenomena but remains incomplete. Therefore, it is of utmost importance to verify its foundational theories as precisely as possible in all their facets, especially in extreme situations. The ALPHATRAP experiment is a dedicated cryogenic Penning-trap apparatus, designed for this exact purpose. At ALPHATRAP it is possible to measure the g -factor of bound electrons ranging from light molecular hydrogen ions to heavy highly charged ions using widely applicable nondestructive single ion spectroscopy techniques [1]. Here, I will present the latest measurements of the bound electron g factor in H-like, Li-like, and B-like tin ion ($Z=50$) with 0.5 parts-per-billion precision. There, extreme electric field strength up to $1\text{E}15\text{ V/cm}$ act on the electron, magnifying QED effects and allowing to test them to highest precision via the comparison with theory predictions [2,3].

Furthermore, I will show the recent spectroscopy results regarding the hyperfine spectroscopy of a single HD^+ ion, which probes the fundamental spin-spin interaction theory [4]. The precise knowledge of the hyperfine structure of HD^+ is very important since it contributes to the determination of the fundamental masses of the electron, proton and deuteron via high precision HD^+ laser spectroscopy results [5]. Further measurements are particularly valuable to resolve the current 9-sigma discrepancy between hyperfine theory and experiment [6]. Finally, I will present the current status of the rovibrational laser spectroscopy on a single trapped HD^+ , which is essential for future high-precision matter-antimatter comparisons [7].

[1] Sturm et al. *Eur. Phys. J. Spec. Top.* **227**, 1425 (2019).

[2] Morgner et al. *Nature* **622**, 5357 (2023).

[3] Morgner et al. *Phys. Rev. Lett.* **134**, 123201 (2025).

[4] König et al. *Phys. Rev. Lett.* **134**, 163001 (2025).

[5] Karr and Koelemeij *Mol. Phys.* **121** 2216081 (2023).

[6] Haidar et al. *Phys. Rev. A* **106**, 042815 (2022)

[7] Myers *Phys. Rev. A* **98**, 010101 (2018).

#B74: Fundamental physics, precision measurements, atom interferometry and atomic clocks

A definition of the SI second based on several optical transitions

Jérôme Lodewyck

LTE / LNE-OP

Optical clocks have now surpassed the Cs based primary frequency standards by two orders of magnitude. The working groups of the Consultative Committee for Time and Frequency are now evaluating the different options for the redefinition, expected to take place in the early 2030s. In this paper, I present one of these options, that proposes to define the second based on the average of several transitions. Such a definition would allow to take advantage of the variety of optical frequency standards available today. We show how this definition can be realized, and give an analysis of its advantages and drawbacks.

#B75: Quantum technologies, quantum optics, cavity QED, quantum information

The Cumulant Expansion Approach: the Good, the Bad and the Ugly

Johannes Kerber; Laurin Ostermann; Helmut Ritsch

Institut für Theoretische Physik, Universität Innsbruck

The configuration space, i.e. the Hilbert space, of compound quantum systems grows exponentially with the number of its subsystems: its dimensionality is given by the product of the dimensions of its constituents. Therefore a full quantum treatment, in general, is hardly possible analytically and can be carried out numerically for fairly small systems only. Yet, in order to obtain interesting physics, an approximation might very well suffice. One of these approximations is given by the cumulant expansion, where expectation values of products of operators are replaced by products of expectation values of said operators, neglecting higher-order correlations. The lowest order of these approximations is widely known as the mean field approximation and used routinely throughout quantum physics. Despite its ubiquitous presence, a general criterion for its applicability remains to be found. In this paper, we discuss two problems in quantum electrodynamics and quantum information, namely the collective radiative dissipation of a dipole-dipole interacting chain of atoms and the factorization of a bi-prime by annealing in an adiabatic quantum computer. On the one hand, we find smooth behaviour, where the approximation becomes increasingly better with higher orders, while, on the other hand, we are puzzled by completely uncontrolled solutions.

#B76: Quantum technologies, quantum optics, cavity QED, quantum information

Correlated vortex generation in coherent medium

Priyabrata Seth¹; Dipankar Bhattacharyya²; Nawaz S Mallick¹; Sankar De¹

¹ Saha Institute of Nuclear Physics, 1/AF, Bidhannagar, Kolkata 700064, India

² Santipur College, Santipur, Nadia, West Bengal 741404, India

Optical vortices are optical beams characterized by a helical phase structure around their axis, possessing unique properties associated with orbital angular momentum (OAM) and phase singularities. Their significance is growing in both quantum communication and quantum computation due to their ability to encode and process information in higher-dimensional state spaces, expanding beyond traditional binary qubit systems [1].

We have experimentally observed the correlated vortex generation in the presence of a coherent medium. This new field has been generated from an old field applied to the coherent atoms. The uniqueness of this generation is that the new field replicates the helical phase front, carrying the same amount of OAM.

Coherent atoms are generated with a spatially separated ring-shaped (annular) beam. Then those atoms are again exposed under the influence of another beam with photons carrying $+4$

hslash of OAM, positioned at the center of the ring. According to our experimental condition, we have separated two interaction regions, leading to a spatial evolution of the coherence. This spatial evolution of coherent atoms is verified through Ramsey interferometry, confirming the phase coherence dynamics in the system. This spatial evolution is highly sensitive to the magnetic field environment, which determines the frequency of the oscillation of this coherence in the dark region (in between the outer ring beam and the central beam).

This coherent generation is a third-order nonlinear process that requires both high optical power and a higher atomic number density. To achieve the necessary conditions, we used a standard vapor cell, which was heated to increase the atomic density and enhance the interaction strength.

We have used the well-known tilted lens detection method [2] to verify the generation and transfer of the OAM of the generated light. We also did the intensity correlation measurements between the generated beam and the applied beam by means of two identical photo detectors. We also have analyzed the sensitivity of the generation against the phase of initial coherence.

[1] Y. Shen, *et al.*, Light: Science & Applications 8, 90 (2019)

[2] P. Vait, *et al.*, Physics Letters A 377, 1154-1156 (2013)

#B77: Quantum technologies, quantum optics, cavity QED, quantum information

Quantum Metrology in the Ultrastrong Coupling Regime of Light-Matter Interactions: Leveraging Virtual Excitations without Extracting Them

Karol Piotr Gietka

Universität Innsbruck

Virtual excitations, inherent to ultrastrongly coupled light-matter systems, induce measurable modifications in system properties, offering

a novel resource for quantum technologies. In this work, we demonstrate how these virtual excitations and their correlations can be harnessed to enhance precision measurements, without the need to extract them. Building on the paradigmatic Dicke model, which describes the interaction between an ensemble of two-level atoms and a single radiation mode, we propose a method to harness hybridized light-matter modes for quantum metrology. Our results not only highlight the potential of virtual excitations to surpass classical precision limits but also extend to a broad range of ultrastrongly coupled systems.

#B78: Quantum technologies, quantum optics, cavity QED, quantum information

Triggered photons from an ion-mirror system

Giovanni Cerchiari¹; Rainer Blatt²; Thomas Lafenthaler²; Thomas Monz²; Tommaso Faorlin²; Yannick Weiser²

¹ Universität Innsbruck, Universität Siegen

² Universität Innsbruck

We are designing a setup composed of a hollow hemispherical mirror, an active boundary condition and a trapped ion for application in quantum networks. The ion will be held in the focal point of the system so that its spontaneous emission will be controlled both by the hemispherical mirror and by the active boundary condition. The hemispherical mirror will suppress the emission at high angles, whereas the active boundary condition will control dynamically the emission at low angles along the optical axis. The setup aims at increasing the entanglement rate of quantum networks based on free space atoms and may be adapted for deterministic transfer of quantum information between two separated atoms.

#B79: Quantum technologies, quantum optics, cavity QED, quantum information

Quantum information processing and error correction in molecular rotation

Brandon Furey¹; Philipp Schindler¹; Zhenlin Wu¹; Mariano Isaza Monsalve¹; René Nardi²; Andrea Turci¹

¹ Universität Innsbruck

² Universität Innsbruck

The rotation of trapped molecules, with state spaces of larger angular momentum and their relatively large electric dipole moments, could offer a promising platform for quantum technologies and quantum information processing (QIP). To explore the experimental utility of molecules for various quantum applications, we are developing state preparation and coherent control protocols based on quantum logic spectroscopy. This technique maps quantum information from molecular to atomic ions for robust state detection. Beyond state preparation and single molecule control, a key requirement for QIP is the generation of quantum entanglement. We are developing strategies for entangling two molecular ions in their angular momenta.

As these QIP operations are implemented on molecules, environment-induced noise can corrupt the quantum state. Quantum error correction codes that protect quantum information encoded in rotational states of a single molecule have recently been developed [1]. We present a step towards experimental implementation of one family of such codes, namely absorption-emission codes. We construct check and correction operators and then describe and analyze a

measurement-based sequential as well as an autonomous implementation strategy in the presence of thermal background radiation, a major noise source for rotation in polar molecules. The presented strategies and methods might enable robust sensing or even fault-tolerant quantum computing using the rotation of individual molecules [2].

- [1] S.P. Jain et al. *Phys. Rev. Lett.* **133**, 260601 (2024)
 [2] B.J. Furey et al. *Quantum* **8**, 1578 (2024)

#B80: Quantum technologies, quantum optics, cavity QED, quantum information

Gravity in the Cavity: Cavity QED as a quantum simulator for cosmological perturbations

Simon Brunner; Yaser Tavakoli; Farokh Mivehvar; Helmut Ritsch

Universität Innsbruck

Phononic excitations in a Bose-Einstein condensate (BEC) exhibit dispersion relations analogous to those of relativistic scalar fields. It has been demonstrated that these fluctuations can be engineered to serve as quantum simulators for Friedmann–Lemaître–Robertson–Walker (FLRW) cosmologies [1]. We propose utilizing a BEC with long-range interactions induced by an optical cavity as a platform to simulate perturbations to the FLRW metric. Starting from the action describing a two-level cold atomic gas confined in a pumped optical cavity, we derive an analytical framework for long-wavelength excitations above the ground state. In the regime of weak cavity pumping, we identify a mapping between the emergent phononic dynamics and a cosmological spacetime with scalar perturbations.

- [1] Viermann, C. et al. *Nature* **611**, 260–264 (2022).

#B81: Quantum technologies, quantum optics, cavity QED, quantum information

Development of ion trap technologies for studying mesoscopic quantum states

Samuel J. M. White¹; Jean Paul Louys Sansó¹; Stefan Schrems²; Lorenz Hummer²; Eric S. Endres¹; Dmitry S. Bykov¹; Markus Arndt²; Tracy E. Northup¹; Roland Wester¹

¹ Universität Innsbruck
² Universität Wien

Nanoparticles have emerged as a promising platform for performing macroscopic quantum experiments and probing the quantum-classical boundary. Recent advances in the field include the motional ground state cooling of gigadalton (GDa) mass silica nanoparticles [1] and the demonstration of matter-wave interferometry with >25 kDa molecules [2]. We aim to trap, image and cool nanoparticles in the 1–10 MDa mass range in preparation for conducting matter-wave interferometry experiments in a new regime with a quantum macroscopicity several orders of magnitude larger than the state of the art. These developments will open the door to study the internal complexity of a range of additional biological and special-purpose particles which may provide novel functionalities and advantages for quantum sensing techniques.

Particles in this mass range provide new challenges in loading, trapping, cooling and detection. We will present our current progress in the development and testing of a special-purpose ion trap and detection scheme utilising recent advancements in the area [3] and which we will integrate with an electrospray ionisation (ESI) ion source. This loading scheme will allow us to quickly change the ions being studied and has been demonstrated to facilitate fragment-free ionisation of complex high-mass molecules [4, 5].

- [1] U. Delić, M. Reisenbauer, K. Dare, D. Grass, V. Vuletić, N. Kiesel and M. Aspelmeyer, Cooling of a levitated nanoparticle to the motional quantum ground state, *Science*, 2020, **367**, 892–895.

- [2] Y. Y. Fein, P. Geyer, P. Zwick, F. Kialka, S. Pedalino, M. Mayor, S. Gerlich and M. Arndt, Quantum superposition of molecules beyond 25 kDa, *Nat. Phys.*, 2019, **15**, 1242–1245.

- [3] D. S. Bykov, L. Dania, F. Goschin and T. E. Northup, 3D sympathetic cooling and detection of levitated nanoparticles, *Optica*, 2023, **10**, 438–442.

- [4] K. Geistlinger, F. Dahlmann, T. Michaelsen, M. Ončák, E. Endres and R. Wester, Multiple helium tagging and OH vibrational spectroscopy of cold protonated glycine ions, *J. Mol. Spectrosc.*, 2021, **379**, 111479.

- [5] C. Sprenger, S. J. M. White, M. Westermeier, F. Dahlmann, M. Ončák, E. S. Endres and R. Wester, UV spectroscopy of [dAMP–H]⁺ at 3 K, (in preparation).

#B82: Quantum technologies, quantum optics, cavity QED, quantum information

Progress toward Neutral Atom Array Processor

Jinyu Zhou; Kai Xiang Lee

Centre for Quantum Technologies

We are developing digital and analog quantum processors based on Cs neutral atom arrays. We plan to realize defect-free atomic arrays with more than 200 qubits. The atom array is expected to have state-of-the-art performance such as >1s qubit coherence time, >95% SPAM fidelity, > 99.9% and > 99% single and two qubit gate fidelity, respectively. Currently we have made some progress in system design, vacuum system, 2D MOT and tweezer generation. On the theory side, we are developing quantum error correction codes and quantum simulation protocols that would be implemented on our quantum processors.

#B83: Quantum technologies, quantum optics, cavity QED, quantum information

From Quantum Statistics to Work: The Pauli Engine and Beyond

Keerthy Menon¹; Thomas Fogarty¹; Eloisa Cuestas²; Jennifer Koch³; Sian Barbosa³; Eric Lutz⁴; Artur Widera³; Thomas Busch¹

¹ OIST Graduate University
² Forschungszentrum Jülich
³ RPTU Kaiserslautern-Landau
⁴ University of Stuttgart

Heat engines convert thermal energy into mechanical work and have been extensively studied in the classical and quantum regimes. In the

quantum domain, however, nonclassical forms of energy exist, which are distinct from traditional heat and which can also be harnessed to generate work in cyclic engine protocols.

We introduce the concept of the Pauli engine: a novel quantum many-body engine powered by the energy difference between fermionic and bosonic ultracold particle ensembles, arising from the Pauli exclusion principle. The distinct quantum statistics lead to a redistribution of population across energy levels, enabling engine cycles that replace traditional heat strokes in the quantum Otto cycle. This concept has recently been realized experimentally in the BEC-BCS crossover regime [1].

Building on this idea, we also present several concepts for hybrid quantum-classical engines, where a change in quantum statistics is implemented either during the adiabatic work strokes or the isochoric heat strokes. While the Pauli engine alone demonstrated high efficiency, we show that combining quantum and classical effects can further enhance both efficiency and work output. All cycles are discussed in the context of ultracold atomic gases, which are well suited for their experimental realisation.

[1] J. Koch, K. Menon, E. Cuestas, S. Barbosa, E. Lutz, T. Fogarty, Th. Busch, A. Widera, *Nature* 621, 723 (2023).

#B84: Quantum technologies, quantum optics, cavity QED, quantum information

2D Coulomb Crystal Vibrational Dynamics for Qubit Application

Niklas Lausti; Vineet Kumar; Michal Hejduk

Charles University

Trapped ions are one of the most promising platforms for a large-scale quantum computer. For this purpose, they are usually cooled to temperatures at millikelvin range, where they form Coulomb crystals. A trapped-ion quantum computer based on a linear crystal of 24 ions has been previously demonstrated [1]. However, the length of a linear crystal creates increasing challenges for production of a computer with a higher number of ions [2]. One solution could be a platform of several traps and transport of ions between them by QCCD architecture [3], but this approach requires complicated electric circuitry. A trap array without ion transport between traps has been also suggested [4], but it has a drawback of low coupling rates between the ions. An alternative idea is to confine the ions to a single multidimensional crystal in a point Paul trap. Unfortunately, we are not aware of any extensive study for defining the vibrational modes of ion crystals in a realistic point Paul trap design.

We present a method for finding the vibrational modes based on ion trajectories from FEM simulations and their frequency analysis. The simulations have been made by using the oscillating electric field of our coaxial Paul trap, also solved by FEM. We successfully test the method for finding in-plane vibrational modes for crystals from one to seven ions and comparing it with reference data [5]. We also evaluate the melting points of such crystals, in order to prevent geometric changes. The results are expected to contribute to the future development of qubits in our laboratory, as well as offer guidelines for comparable work with other Paul traps.

References

- [1] I. Pogorelov et al., *PRX Quantum* 2, 020343, (2021)
- [2] P. Murali et al., *IEEE Micro* 40, 73–80, (2020)
- [3] J. M. Pino et al., *Nature* 592, 209–213, (2021)
- [4] P. C. Holz et al., *Adv. Quantum Technol.* 3, 2000031, (2020)
- [5] K. Nelissen et al., *Phys. Rev. E* 73, 016607, (2006)

Poster Session C

#C1: Atomic and molecular spectroscopy, photo-induced processes

Cold electronic spectroscopy of metal phthalocyanine cations

Lisa Ganner; Gabriel Schöpfer; Florian Foitzik; Stefan Bergmeister; Milan Ončák; Elisabeth Gruber

Institute for Ion Physics and Applied Physics, Universität Innsbruck

The increasing interest in photoactive organic molecules for solar energy conversion systems, photocatalysis, and photodynamic therapy, requests a deep understanding of their photophysical and photochemical properties and how the microenvironment affects them. Metal phthalocyanines (MPcs), a class of highly conjugated macrocyclic compounds, are particularly promising due to their strong light absorption, tunable electronic properties, and high chemical stability.

In this study, we present experimental and theoretical spectroscopic investigations of metal phthalocyanine cations in the UV/Vis wavelength range, focusing on the influence of the central metal atom on electronic transitions. Using helium nanodroplets as a cryogenic environment, we form MPc monomer cations in their electronic ground states. For spectroscopic studies, the molecular ions are extracted from the helium matrix with a few helium atoms still attached, serving as gentle tag. Upon photoabsorption, the helium evaporates, and the resulting photofragments are analysed via time-of-flight mass spectrometry [1]. In addition, we exploit the advantages of helium nanodroplets to form tailored cluster ions via sequential pick-up, enabling the controlled attachment of individual atoms and molecules such as water to investigate environmental effects [2]. We present high-resolution laser absorption spectra of various MPcs, show that the hydration of the ions has only a minor influence on the electronic spectra, and discuss the advantages of our experimental method.

References:

- [1] S. Bergmeister et al., *Rev. Sci. Instrum.* **94**, 055105, (2023)
- [2] S. Bergmeister et al., *Adv. Sci.* **11**, 2307816, (2024)

#C2: Atomic and molecular spectroscopy, photo-induced processes

Quantum Optimal Control of Molecular Orientation

Juan José Omiste Romero

Universidad Complutense de Madrid

Precise molecular orientation is crucial for optimizing chemical reaction efficiency and enabling distortion-free measurements in the molecular frame [1,2]. We propose using Quantum Optimal Control theory to orient any molecular axes along any laboratory direction, extending previous results on ground-state molecular rotational states [3,4]. Specifically, we focus on highly rotating molecular states, known as superrotors. These states exhibit stable alignment on a plane due to centrifugal forces, making them promising candidates for precise control of the non-aligned molecular axis.

Beyond controlling molecular orientation, we extend our framework to manipulate spin states [5] in molecular spin chains, providing a versatile tool for quantum information processing and transport.

- [1] H. Stapelfeldt and T. Seideman, *Rev. Mod. Phys.* **75**, 543–557 (2003)
- [2] Y. Sheng, Y. Yan, P. F. Cui, J. Yu, S. Chai and S. L. Cong, *Chem. Phys.* **563**, 111690 (2022)
- [3] L. H. Coudert, *J. Chem. Phys.* **146**, 024303 (2017)
- [4] R. González-Férez, and J. J. Omiste, *Phys. Chem. Chem. Phys.* **26**, 4533–4540 (2024)
- [5] A. Castro, A. García Carrizo, S. Roca, D. Zueco, and F. Luis, *Phys. Rev. Appl.* **17**, 064028 (2022)

#C3: Atomic and molecular spectroscopy, photo-induced processes

Photodetachment vibronic dynamics using nonlocal discrete-state-in-continuum model

Jan Zlatník; Martin Čížek; Mattias Bertolino

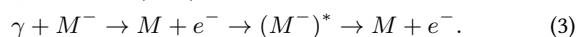
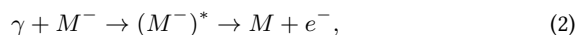
Charles University, Faculty of Mathematics and Physics, Prague

Synopsis In this work, we demonstrate how the discrete-state-in-continuum model, previously used for electron-molecule collisions, can be generalized to treat the vibronic dynamics in electron photodetachment from molecular anions. The theory is tested on models motivated by diatomic molecules, exploring phenomena known from electron-molecule collisions, such as boomerang oscillations, Wigner cusps, and vibrational Feshbach resonances.

We extend the nonlocal discrete-state-in-continuum model based on the projection-operator formalism, previously successfully applied to inelastic electron-molecule collisions [1], to describe electron photodetachment from molecular anions. A crucial aspect of this process is the absorption of a photon by a molecular anion in its ground state, leading to the formation of a metastable molecular anion, which then undergoes vibronic dynamics before decaying into the electron molecule scattering continuum. By tracking the energy of the released electrons as a function of photon energy, a 2D spectrum can be obtained, similar to electron energy loss spectroscopy (EELS) [2], which serves as a suitable experimental method for studying these processes.

In the preprint [3], we present the theoretical framework and apply it to a simplified model of a diatomic molecular anion inspired by LiH^- . In later research, we vary the parameters of the diatomic model in an attempt to observe additional resonance phenomena known from electron molecule collisions, including boomerang oscillations, Wigner cusps, and vibrational Feshbach resonances, with preliminary results available in [4]. Furthermore, we implement two approximations: the adiabatic nuclei approximation and the local complex potential approach. We analyze the limits of these approximations and their applicability to describe different phenomena.

The photodetachment cross-section amplitude shows contributions from three competing processes: direct background detachment (1), resonant autodetachment (2), and temporary photodetachment followed by reattachment and subsequent autodetachment (3):

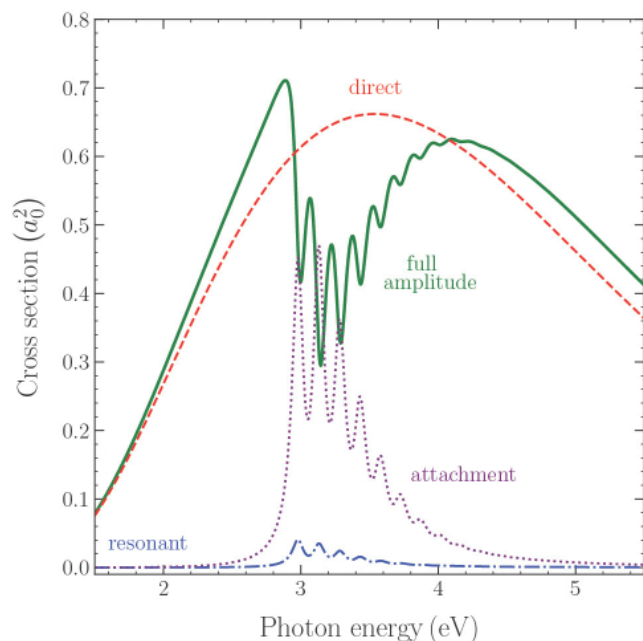


The relative contribution of these mechanisms is illustrated in the figure on a model exhibiting boomerang oscillations.

Fig.: Photodetachment cross-section as a function of photon energy, illustrating contributions from different processes in a model exhibiting boomerang oscillations.

References

- [1] Domcke W., *Phys. Rep.* **208** 97–188, (1991)
- [2] Anstötter C. S. et al, *Phys. Rev. Lett.* **124**, 203401, (2020)
- [3] Čížek M., *arXiv* [arXiv:2309.05830](https://arxiv.org/abs/2309.05830), (2023)



[4] Zlatník J., *Bc thesis, Charles University, Prague*
[hdl:20.500.11956/191309](https://hdl.handle.net/20.500.11956/191309), (2024)

#C4: Atomic and molecular spectroscopy, photo-induced processes

Fourier-limited electronic transitions in surface-adsorbed quantum emitters

Alexey Shkarin¹; Masoud Mirzaei¹; Burak Gurlek¹;
 Ashley Shin¹; Johannes Zirkelbach¹; Irena
 Deperasinska²; Boleslaw Kozankiewicz²; Tobias Utikal¹;
 Stephan Goetzinger¹; Vahid Sandoghdar¹

¹ Max Planck Institute for the Science of Light

² Institute of Physics, Polish Academy of Sciences

Organic dye molecules doped in organic host crystal provide an exquisite platform for quantum optics because they can reach Fourier-limited spectra at low temperatures. This is in large part due to the highly ordered and stable crystal structures, which provide a low-noise environment, thus minimizing spectral diffusion and dephasing. Many important fundamental studies and technological applications, however, require quantum emitters to be exposed on surfaces. To date, Fourier-limited spectra have remained elusive for quantum emitters on surfaces. In fact, the general wisdom expects surfaces to be intrinsically unsuitable for such studies because they contain defects and contaminants.

In our recent work, we show that it is possible to achieve Fourier-limited electronic transitions for molecules on pristine surfaces of an organic crystal. We have developed a novel sample preparation method, where molecules are sublimated onto the pristine surface of an organic crystal at cryogenic temperatures. We provide detailed quantitative studies on the resulting inhomogeneous broadening at the ensemble level and the behavior of the homogeneous linewidth at the single-molecule level. By comparing the spectral properties of the same molecular species in the gas phase with its properties on the surface and bulk, we shed light on several fundamental aspects of guest-host interactions. This study constitutes an important step in combining high-resolution spectroscopy and quantum optical studies

with techniques such as AFM and STM, which provide direct access to individual molecules.

#C5: Atomic and molecular spectroscopy, photo-induced processes

Laser spectroscopy of the X-A transition in CO⁺⁺

Xavier Huet¹; Antoine Aerts¹; Nathalie Vaeck¹;
 Xavier Urbain²; Matthieu Génévriez²

¹ Université Libre de Bruxelles

² Université catholique de Louvain

Doubly charged molecular ions are elusive species that, despite their role in plasmas [1], have rarely been spectroscopically characterized. We report the first study by laser spectroscopy of the X(³Π_Ω)-A(³Σ⁺) transition of the CO⁺⁺ ion. Experimentally, a fast beam of CO⁺⁺ ions was produced from a plasma ion source. In the ground electronic state, all vibrational levels except the ground state and the first excited state are short lived. Therefore, despite the high temperature of the ion source, only those ions with $v = 0, 1$ are present in the beam. The beam is then intersected, at a small angle, by a laser beam resonant with rovibrational transitions from the X to the A state. In the A state, the ions rapidly predissociate and Coulomb explode into C⁺ and O⁺ fragments whose kinetic energies are known. Excitation spectra are recorded in a background-free manner by scanning the laser while detecting, in coincidence, the C⁺ and O⁺ fragments with the appropriate energy. Experimental investigations are assisted by accurate ab-initio calculations of the potential-energy curves of twelve low-lying states of CO⁺⁺ with the multi-reference configuration interaction method. The nonadiabatic spin-orbit couplings are also calculated and used, together with the potential-energy curves, to determine the energies of the rovibrational levels and their lifetimes with a complex-scaling-based method.

With this approach we measured the spectra of the X($v' = 0, 1$)-A($v = 0 - 2$) vibronic transitions. The resolution achieved ($\sim 5 \text{ cm}^{-1}$) represents a 15-fold improvement compared to previous studies [2]. The rotational envelopes of the vibronic spectra confirm the theoretical values of the rotational constants, and the spin-orbit splitting of the X state is fully resolved and characterized for the first time. We also extract from our spectra and calculations an accurate set of spectroscopic constants of the X and A states of CO⁺⁺. These results provide a benchmark for understanding doubly-charged molecular ions of atmospheric relevance.

[1] Thissen et al., *Phys. Chem. Chem. Phys.* **41**, 18264 (2011)

[2] Penent et al., *Phys. Rev. Lett.* **81**, 3619 (1998)

#C6: Atomic and molecular spectroscopy, photo-induced processes

Vibrational Induced Molecular Magnetism: A Theoretical Perspective

Matthias Diez; Johannes K. Kronendorfer; Andreas W.
 Hauser

Graz University of Technology, Institute of Experimental Physics

First experimental observations and theoretical insights into rotational and vibrational magnetism in molecules date back more than 50 years, but a comprehensive framework for vibrationally induced magnetism

remains elusive. Analogous to magnetic effects induced by molecular rotation, twofold degenerate molecular vibrations, when excited with a $\pi/2$ phase shift, induce rotational motions of the nuclei, generating vibrational magnetic moments and intramolecular magnetic fields. We derive a consistent theoretical framework for these effective couplings, unifying nuclear spin-vibration and nuclear spin-rotation coupling. Calculations on benchmark molecules, which are known to show a vibrational Zeeman effect, demonstrate non-negligible vibrationally induced chemical shifts, and therefore a non-trivial intermolecular field geometry. Given the growing interest in molecular magnetism, particularly based on transition-metal complexes, we focus on metal phthalocyanines — a versatile, planar, macrocyclic molecules with a central metal ion — to identify configurations that maximize vibrationally induced magnetic effects.

#C7: Atomic and molecular spectroscopy, photo-induced processes

Highly oriented pyrolytic graphite chemical bonding structure after gallium implantation

A. Sulyok¹; G.Z. Radnóczy¹; H.A.A. Abdelbagi²; J.B. Malherbe³; Károly Tokesi⁴; T.A.O. Jafer³

¹ HUN-REN Centre for Energy Research, Institute of Technical Physics and Materials Science, Budapest, Hungary

² Physics Department, University of Zululand, KwaDlangezwa, 3886, South Africa

³ Physics Department, University of Pretoria, Hatfield, Pretoria, South Africa

⁴ HUN-REN Institute for Nuclear Research

Highly oriented pyrolytic graphite (HOPG) structural changes caused by gallium (Ga) implantation at room temperature were investigated. To monitor structural changes in the samples after implantation, Raman spectroscopy was used. SRIM (Stopping and Range of Ions in Matter 2013) software was applied to determine the depth profiles of Ga implanted at different energies and the degree of damage in HOPG after implanting Ga. Accordingly, SRIM and Raman results suggest that amorphizing our HOPG sample requires a dpa above 4 dpa, which is much higher than previously reported (0.20 dpa).

Acknowledgments

The work was supported by the Bilateral relationships between South Africa and Hungary in science and technology (S&T) under the project number 2019–2.1.11-TET-202000123

#C8: Atomic and molecular spectroscopy, photo-induced processes

Calculated absorption and circular dichroism spectra of TPPS4 molecular aggregates

Laura Baliulyte¹; Eimantas Urniezius¹; Vytautas Bubilaitis¹; Mindaugas Macernis¹; Lorenzo Cupellini²; Darius Abramavicius¹

¹ Institute of Chemical Physics, Faculty of Physics, Vilnius University

² Department of Chemistry and Industrial Chemistry, University of Pisa

Recently there has been growing interest in TPPS4 for applications in photodynamic therapy as photosensitizer [1]. The monomers of this porphyrin efficiently self-associate into H- and J-aggregates in aqueous media. It is not fully understood what kind of TPPS4 configurations are building blocks of molecular aggregates. For these reasons,

the aim of this study is to determine tetramers and calculate their absorption and circular dichroism (CD) spectra.

First of all, quantum mechanical (QM) calculations were performed on geometry optimizations of the structures of TPPS4 zwitterionic monomers. Two different types of the zwitterionic form of the TPPS4 molecules were considered with respect to position of SO₃H protonized groups: either these groups are opposite (Z1 monomer) or adjacent (Z2 monomer). QM calculation were performed using the DFT B3LYP/6-311G(d,p) basis set and polarizable continuum model (PCM) methods. The Gaussian 16 program was used. The next step was to take parameters from the General Amber force field (GAFF). It was also adjusted several parameters of monomers. Molecular mechanics (MM) geometry optimization was also performed. The second step was to construct Z1 and Z2 tetramers. The obtained tetramers were solvated with water boxes. Then molecular dynamics (MD) simulation was performed with AMBER 22 program.

Theoretical calculations of the TPPS4 tetramer's absorption and CD spectra were performed for Z1 and Z2 tetramers. The Frenkel excitonic model was used for this task as the electrons are localized to each molecule so we were able to treat each excitation as an exciton. These calculations were performed by associating 4 optical transitions to each molecule constituting the aggregate, which are in turn characterized by their respective transition energies for the Q and B band and an optical transition dipole moment vector for each transition (μ): i, j, k and l, the first two vectors corresponding to the Q band and vectors three and four to the B band. Each vector's coordinates were associated with the coordinates of each molecule's central nitrogen atoms. The tetramer's spectral density was calculated and then averaged for all 5000 frames of the simulation and normalized to a maximum of 1. It was determined two Z1 and Z2 linear tetramers. A comparison was performed of Z1 and Z2 tetramers absorption spectra with the measured spectra from the previous published article [2]. Our analysis of results demonstrates that larger peak shift of Z1 tetramer's spectra are more similar to the experimental data, however other configurations can be possible as well.

References

- [1] Q. Xiao, J. Wu, X. Pang, Y. Jiang, P. Wang, A. W. Leung, L. Gao, S. Jiang, and C. Xu, "Discovery and development of natural products and their derivatives as photosensitizers for photodynamic therapy," *Curr. Med. Chem.* 25(7), 839–860 (2018).
- [2] L. Baliulyte, D. Abramavicius, S. Bagdonas, A. Kalnaityte, V. Poderys, R. Rotomskis, and V. Barzda, "Comparative quantum chemical and spectral characterization of meso-tetra (4-sulfonatophenyl) porphine forms as seeds for J- and H-aggregates," *AIP Advances* 13(10) (2023).

#C9: Atomic and molecular spectroscopy, photo-induced processes

Atomic data for Os VI spectral lines of interest to nuclear fusion research from independent computational approaches

Maxime Brasseur; Pascal Quinet; Patrick Palmeri

Université de Mons

It is now well established that the ITER Tokamak divertor will be made of tungsten (Z=74). During nuclear fusion operations, the divertor will endure some of the harshest conditions in the reactor. Thus, under neutron bombardment, tungsten will undergo nuclear transmutation, forming other elements, including osmium (Z=76). On the one hand, these impurities will contribute to the radiation losses and, on the other, they could allow to diagnose the fusion plasma in terms of impurity influx, temperature and density. Therefore, knowledge of the radiative data for Os ions is of great interest. The present work is focused on Os VI for which new transition probabilities were determined using two independent methods, namely the pseudo-relativistic Hartree-Fock including core-polarization effects (HFR+CPOL) and the fully relativistic Multiconfiguration Dirac-Hartree-Fock (MCDHF) ap-

proaches. This allowed us to provide gA-values for 367 experimentally observed lines in Os VI in the wavelength range between 438.720 and 1486.275 Å, the quality of the new data being assessed through detailed comparisons between the results obtained using both computational approaches.

#C10: Atomic and molecular spectroscopy, photo-induced processes

Bottom-up Analysis of Ro-Vibrational Helical Dichroism

Mateja Hrast¹; Georgios M. Koutentakis¹; Mikhail Maslov¹; Mikhail Lemeshko²

¹ IST Austria

² Institute of Science and Technology Austria

Enantiomer-selective methods - the separation of non-superimposable mirror-image chiral molecules - is critical for many industries relying on chiral purity. Traditional methods like circular dichroism exploit the spin angular momentum of light but their sensitivity is limited by the inherent molecular properties. Orbital angular momentum (OAM) in structured light offers a promising alternative through helical dichroism (HD), hypothesized to arise from electric-dipole-electric-quadrupole interactions. We present a rigid theoretical framework for the analysis of HD, based on molecular symmetries and rotational selection rules [1]. Using our recently developed model of molecule-light interaction Hamiltonian [2] we analyse how a chiral molecule interacts with OAM-carrying light and elucidate the microscopic mechanisms of OAM transfer to the molecular rotation. Going beyond the conventional assumptions on HD, we uncover that paraxial OAM-carrying beams, such as Laguerre-Gaussian modes, cannot transfer OAM to molecular rotations. In fact, HD only emerges from spin-orbit coupled light, such as tightly focused beams. Strikingly, even beams without OAM away from the focus, induce enantiomer-sensitive absorption profiles that can be attributed to HD. Our findings redefine the conditions for observing HD, motivating the reassessment of prior experiments and guiding future designs for chiral sensing using structured light.

[1] M. Hrast, G. M. Koutentakis, M. Maslov, and M. Lemeshko, Bottom-up Analysis of Ro-Vibrational Helical Dichroism, (*Manuscript in preparation*).

[2] M. Maslov, G. M. Koutentakis, M. Hrast, O. H. Heckl, and M. Lemeshko, Theory of angular momentum transfer from light to molecules, *Phys. Rev. Res.* **6**, 033277 (2024).

#C11: Atomic and molecular spectroscopy, photo-induced processes

Testing strong-field QED to second-order in highly correlated berylliumlike Pb⁷⁸⁺ by electron-ion collision spectroscopy

Stefan Schippers¹; Carsten Brandau²; Sebastian Fuchs¹; Michael Lestinsky²; Shuxing Wang¹; Chunyu Zhang³; Nigel Badnell³; Alexander Borovik¹; Mike Fogle⁴; Volker Hannen⁵; Zoltán Harman⁶; Pierre-Michel Hillenbrand²; Esther Babette Menz²; Yanning Zhang⁷; Zoran Andelkovic²; Frank Herfurth²; Regina Heß²; Anton Kalinin²; Christophor Kozhuharov²; Claude Krantz²; Sergey Litvinov²; Bernd Lorentz²; Uwe Spillmann²; Markus Steck²; Gleb Vorobyev²; Dariusz Banaś⁸; Stephan Fritzsche⁹; Eva Lindroth¹⁰; Xinwen Ma¹¹; Alfred Müller¹; Reinhold Schuch¹⁰; Andrey Surzhykov¹²; Martino Trassinelli¹³; Ken Ueberholz¹⁴; Christian Weinheimer¹⁴; Thomas Stöhlker⁹

¹ I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

² GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

³ Department of Physics, University of Strathclyde, Glasgow G4 0NG, UK

⁴ Department of Physics, Auburn University, Alabama 36849, USA

⁵ Institut für Kernphysik, Universität Münster, 48149 Münster, Germany

⁶ Max-Planck-Institut für Kernphysik, 69117 Heidelberg, Germany

⁷ School of Science, Xi'an Jiaotong University, Xi'an 710049, China

⁸ Institute of Physics, Jan Kochanowski University, 25-406 Kielce, Poland

⁹ Helmholtz-Institut Jena, 07743 Jena, Germany

¹⁰ Department of Physics, Stockholm University, AlbaNova, 10691 Stockholm, Sweden

¹¹ Institute of Modern Physics, Chinese Academy of Sciences, 730000 Lanzhou, China

¹² Physikalisches-Technische Bundesanstalt, 38116 Braunschweig, Germany

¹³ Institut des NanoSciences de Paris, CNRS, Sorbonne Université, 75005 Paris, France

¹⁴ Institut für Kernphysik, Universität Münster, 48149 Münster, Germany

Using the experimental technique of electron-ion collision spectroscopy at the electron cooler of the heavy-ion storage ring CRYRING@ESR [1] we have measured merged-beams rate coefficients for electron-ion recombination of berylliumlike Pb⁷⁸⁺ ions. In the electron-ion collision energy range 12–16.5 eV, we have observed $2s2p\ (^3P_1)\ 19l_j$ dielectronic recombination (DR) resonances associated with a $2s^2\ ^1S_0 \rightarrow 2p2p\ ^3P_1$ core excitation and a simultaneous capture of the initially free electron into the $n = 19$ shell of the boron-like Pb⁷⁷⁺ product ion. A careful analysis of the systematic experimental errors reveals that the uncertainty of the measured resonance positions amounts to ± 30 meV. This uncertainty is lower than the theoretical uncertainty of the calculation of the $2s^2\ ^1S_0 \rightarrow 2p2p\ ^3P_1$ excitation energy by Malyshev et al. [2]. By considering second order QED effects and electron-electron correlation effects, which are particularly strong in berylliumlike ions, these authors obtained $E_{\text{exci}} = 244.942(52)$ eV. Within the uncertainties this agrees with our experimental finding [3], which thus constrains second order strong-field QED.

This research was supported by the ErUM-FSP T05 “APPA” (BMBF grant nos. 05P24RG2, 05P24SJA, 05P21PMFA1, 05P21RGFA1, 05P21SJFAA, <https://fsp-appa.fair-center.eu>).

[1] C. Brandau et al., *Chin. Phys. C* (2025), <https://doi.org/10.1088/1674-1137/adbf81>.

[2] A. Malyshev et al. *Phys. Rev. A* **110**, 062824 (2024), <https://doi.org/10.1103/PhysRevA.110.062824>.

[3] S. Schippers et al., Phys. Rev. Lett. submitted, <https://arxiv.org/abs/2502.15433>.

#C12: Atomic and molecular spectroscopy, photo-induced processes

Multiple photoionization of singly charged lanthanum ions

Alfred Müller¹; Aloka Kumar Sahoo²; F. Trinter³; Jörn Seltmann⁴; Michael Martins⁵; Michel Döhring⁶; Mirko Looshorn⁷; Pierre-Michel Hillenbrand⁸; Shuxing Wang⁹; Simon Reinwardt⁵; Stefan Schippers¹⁰; Stephan Fritzsche¹¹

¹ Justus-Liebig-Universität Gießen

² HI Jena

³ Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

⁴ DESY

⁵ DESY, Uni Hamburg

⁶ JLU Gießen

⁷ Uni Gießen, Helmholtz Forschungsakademie Hessen für FAIR (HFHF), GSI Gesellschaft für Schwerionenforschung, Campus Gießen

⁸ GSI Helmholtzzentrum für Schwerionenforschung GmbH, 64291 Darmstadt, Germany

⁹ I. Physikalisches Institut, Justus-Liebig-Universität Gießen, 35392 Giessen, Germany

¹⁰ Justus-Liebig-Universität Gießen, I. Physikalisches Institut

¹¹ Helmholtz-Institut Jena, 07743 Jena, Germany

Using the photon-ion merged-beams technique at a synchrotron light source, we have measured relative cross sections for double and up to tenfold photoionization of La^+ ions in the energy range 820–1400 eV where resonances and thresholds occur that are associated with the excitation or ionization of one M-shell electron. The normalization of the sum of the measured partial cross sections to the absolute photoabsorption cross section of La allows the transformation of the relative cross sections into absolute cross sections.

In 2017, the LIGO/Virgo collaboration detected the first gravitational-wave signal from the merger of a neutronstar binary. Less than two seconds later, a network of telescopes detected a short gamma-ray burst, followed by a longer optical “afterglow” powered by the radioactive decay of the neutron-rich material ejected in the merger, i.e., a kilonova. The kilonova light-curves potentially reveal the abundances of the heavy chemical elements that are produced in the preceding violent neutron-star merger events [1,2].

In order to be able to reliably infer elemental abundances from the astronomical observations, absolute cross sections are required for the basic atomic processes that occur in the afterglow. So far, local thermodynamic equilibrium (LTE) conditions have been assumed in the astrophysical modelling of kilonovae [1,2], which certainly is an oversimplification given the highly dynamic and transient nature of the phenomenon. Any future more accurate non-equilibrium modelling will have to rely on accurate atomic cross sections, which generally cannot be easily calculated (if at all) to a sufficient precision for the heavy many-electron ions of interest.

The present experiments were carried out at the photon-ion merged-beams setup PIPE [3], a permanently installed end-station of the PETRA III photon beamline P04, using already previously established experimental procedures (see e.g. [4]). A beam of La^+ -ions was extracted from a Penning ionization source and merged with the P04

photon beam. Relative yields of multiply charged La^{q+} reaction products with $3 \leq q \leq 11$ were recorded as functions of photon energy over the energy range 800–1400 eV.

References

[1] Kasen D et al. 2017 Nature 551 80

[2] Watson D et al. 2019 Nature 574 497

[3] Schippers S and Müller A 2020 Atoms 8 45

[4] Schippers S et al. 2017 Astrophys. J. 849 5

#C13: Atomic and molecular spectroscopy, photo-induced processes

Infrared absorption spectroscopy of single polyatomic molecular ions

Zhenlin Wu; Brandon Furey; Mariano Isaza Monsalve; Miriam Antonia Kautzky; Andrea Turci; Rene Nardi; Elyas Mattivi; Philipp Schindler

Universität Innsbruck

Molecular spectroscopy studies have been carried out on various diatomic molecular ions co-trapped with atomic ions in ion traps, including CaH^+ , MgH^+ , CaO^+ , HD^+ , N_2^+ and H_2^+ , contributing to fundamental physics research and quantum information processing applications [1–6]. On a similar platform consisting of a single molecular ion co-trapped with one Ca^+ qubit ion, we aim to study polyatomic molecular ions with more complex internal structure than diatomic species. These ions are of particular interest due to, for instance, ultrafast intramolecular vibrational energy redistribution which plays an important role in chemical and biological processes. We plan to perform pump-probe experiments with femtosecond laser pulses on polyatomic molecular ions in our system [7]. The interaction between the pulses and the target molecule can be characterized as single photon absorption events which introduce photon recoils that affects the center-of-mass motion of the two-ion crystal. Making use of the Ca^+ qubit transition, we could probe the change of its motional state and thus detect the single photon absorption events on the molecule [8]. This method is tested on CaOH^+ where we perform vibrational spectroscopy on its O-H stretching mode which has relatively high transition energy and transition dipole moment. With such measurement, we also plan to investigate the possibility of utilizing such intramolecular vibrational mode for rotational state preparation of a polyatomic molecular ion like CaOH^+ with optical pumping via vibrational transitions, as has been demonstrated on diatomic molecular ions with smaller mass [9–10].

[1] F. Wolf et al., Nature 530(7591), 457–460 (2016)

[2] C. W. Chou et al., Nature 545(7653), 203–207 (2017)

[3] M. Sinhal et al., Science 367(6483), 1213–1218 (2020)

[4] S. Alighanbari et al., Nature 581(7807), 152–158 (2020)

[5] D. Holzapfel et al., arXiv:2409.06495 (2024)

[6] L. Qi et al., arXiv:2411.07137 (2024)

[7] P. Schindler, New J. Phys. 21(8), 083025 (2019)

[8] C. Hempel et al., Nature Photonics 7, 630–633 (2013)

[9] P.F. Staunum et al., Nature Phys 6(4), 271–274 (2010)

[10] T. Schneider et al., Nature Phys 6(4), 275–278 (2010)

#C14: Atomic and molecular spectroscopy, photo-induced processes

Transition from Rabi Oscillations to Dynamic Interference seen in the Autler- Townes Doublet: A Multi-Peak Pattern Analysis

Ayoub Ait Elarabi

University of Debrecen

The interaction of intense, short, and (near)resonant laser pulses with a two-level quantum system induces intricate dynamics, characterized by Rabi oscillations (ROs) [1] and dynamic interference (DI) [2], both of which manifest as multi-peak patterns in the photo-electron spectrum. These phenomena, central to strong-field light-matter interactions, often coexist in the Autler-Townes (AT) doublet, making their individual contributions challenging to disentangle. In this study, we investigate the multi-peak structure of the AT doublet through two-photon ionization of hydrogen, employing a combined analytical and numerical framework to uncover its physical origins [3].

Our results reveal that the selective population of dynamically dressed states critically determines the interplay between ROs and DI. Under resonant conditions, ROs dominate, producing quasi-symmetric multi-peak patterns directly correlated with the number of Rabi cycles completed. Conversely, detuned laser pulses suppress ROs, enabling DI to govern the spectrum, resulting in asymmetric, interference-driven modulations. By analyzing the photoelectron spectra and the dynamics of dressed states, we identify distinct spectral signatures marking the transition from RO- to DI-dominated regimes, building on and refining prior insights [2]. These findings deepen our understanding of ultrafast quantum dynamics and pave the way for precise control of light-induced processes in the XUV regime, with potential applications in quantum optics and attosecond science.

[1] S. Nandi et al., Nature 608, 488 (2022).

[2] A. Tóth, S. Borbély, and A. Csehi, Phys. Rev. A 108, L061101 (2023).

[3] A. Ait Elarabi and A. Csehi, Phys. Rev. A 111, 033107 (2025).

#C15: Atomic and molecular spectroscopy, photo-induced processes

Experimental Characterization of All Vibrationally Excited States of the $X^+ \ ^2\Sigma_u^+$ Ground Electronic State of He_2^+

Maxime Holdener; Noah Shahin; Vincent Wirth; Hansjürg Schmutz; Josef Agner; Frédéric Merkt

ETH Zürich

Precise spectroscopic measurements in small molecular systems such as He_2 and He_2^+ are of interest as benchmark for high-accuracy *ab-initio* quantum-chemical calculations in few-electron molecules [1-3]. In the case of He_2^+ , only the lowest ($v^+ = 0 - 2$) [4-5] and highest ($v^+ = 22 - 23$) [6] vibrational levels of the $X^+ \ ^2\Sigma_u^+$ electronic ground state have been characterized experimentally.

We describe methods to access and study all vibrational states of He_2^+ $X^+ \ ^2\Sigma_u^+$ from $v^+ = 0$ to $v^+ = 19$ using a multi-steps excitation scheme.

The approach involves the production of a supersonic beam of He_2 in the long-lived metastable $a^3\Sigma_u^+(v = 0 - 2)$ states using a cryogenic pulsed valve coupled to an electric discharge [7].

A pulsed laser promotes the system to a selected excited rovibrational level of the $c^3\Sigma_g^+$ electronic state with v' and N' in the range 3 - 4

and 0 - 18, respectively.

These states either decay radiatively to vibrationally excited levels of the $a^3\Sigma_u^+$ state or by quantum mechanical tunneling through a barrier in the c-state potential.

A second laser is then employed to induce transitions from these vibrationally excited $a^3\Sigma_u^+(v)$ metastable states to vibrationally excited $\text{He}_2^+ X^+ \ ^2\Sigma_u^+(v^+)$ states with $v^+ \leq 5$.

High-resolution photoelectron spectra of these ionizing transitions are recorded using the technique of pulsed-field-ionization zero-kinetic-energy (PFI-ZEKE) photoelectron spectroscopy.

To study even higher vibrational levels of He_2^+ , the second laser is used to directly photoionize the selected intermediate $c^3\Sigma_g^+(v', N')$ states and record PFI-ZEKE photoelectron spectra of the $X^+ \ ^2\Sigma_u^+(v^+, N^+)$ levels.

With these excitation schemes, spectra of $X^+ \ ^2\Sigma_u^+(v^+, N^+)$ rovibrational levels of He_2^+ could be measured for the first time up to the $v^+ = 19$ rovibrational level.

These new results will be compared with the predictions of *ab-initio* quantum-chemical calculations and are used to determine an empirical potential-energy function for the $X^+ \ ^2\Sigma_u^+$ ground electronic state of He_2^+ that reproduces all experimental data within their experimental uncertainties.

[1] C. F. Chabalowski, J. O. Jensen, D. R. Yarkony, and B. H. Lengsfeld, J. Chem. Phys., 90, 2504-2512 (1989).

[2] D. Ferenc, V. I. Korobov, and E. Matyus, Phys. Rev. Lett., 125, 213001 (2020).

[3] J. Gebala, M. Przybytek, M. Gronowski, and M. Tomza, Phys. Rev. A, 108, 052821 (2023).

[4] M. Raunhardt, M. Schäfer, N. Vanhaecke, and F. Merkt, J. Chem. Phys., 128, 164310 (2008).

[5] L. Semeria, P. Jansen, G.-M. Camenisch, F. Mellini, H. Schmutz, and F. Merkt, Phys. Rev. Lett., 124, 213001 (2020).

[6] A. Carrington, C. H. Pyne, and P. J. Knowles, J. Chem. Phys., 102, 5979-5988 (1995).

[7] M. Motsch, P. Jansen, J. A. Agner, H. Schmutz, and F. Merkt, Phys. Rev. A, 89, 043420 (2014).

#C16: Atomic and molecular spectroscopy, photo-induced processes

An Investigation into CMOS Sensors as Spatially & Spectrally Resolved Soft X-Ray Detectors for Laser Produced Plasma Imaging

Emma Sokell; Fergal O'Reilly; Éanna Donohoe

University College Dublin

CMOS sensors, typically used in smartphone cameras and other commercial applications, have gained recent attention for their potential use in astronomical [1] and biological [2,3] x-ray imaging due to their improved readout speed and resolution, and lower power consumption, noise, and cost compared to their CCD counterparts. This work explores the conversion of two commercial off the shelf CMOS cameras into soft x-ray (SXR) detectors; investigating their spectral resolution, optimizing their sensitivity, and implementing them as laser produced plasma imaging devices.

A Sony IMX477 and a Sony IMX178 were adapted by removal of their glass windows and addition of a free standing 1.4 μm Al filter. Each sensor was spectrally calibrated using known well-defined emission structures of Fe-Zn plasmas in the 600-1200 eV region. In both cases, a linear relationship between photon energy and detected counts was quantified, and with $E/\Delta E > 15$.

We also investigated methods of improving the SXR detection efficiency of the IMX477 detector, particularly in the >600 eV region, by removing polymer layers on the sensor surface, and by thinning the Al filter. The removal of the Bayer layer and microlens array resulted in a 50% increase in sensitivity, but introduced significant non-uniformity. The Al filter was then deposited directly on the CMOS sensor with a thickness of 100 nm through thermal evaporation to extend the spectral sensitivity from 600 eV down to ~ 300 eV.

The work has enhanced our understanding of the behaviour of these cost-effective soft x-ray detectors, although there are still aspects to be explored. We intend to use these sensors in order to spatially map the density of laser plasmas by using soft x-rays as a backlight.

[1] Ogino, Naoki, et al. "Performance Verification of Next-Generation Si CMOS Soft X-ray Detector for Space Applications." *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment*, vol. 987, 2021, article no. 164843.

[2] Alcalde Bessia, Fabricio, et al. "X-ray micrographic imaging system based on COTS CMOS sensors." *International Journal of Circuit Theory and Applications*, vol. 46.10, 2018, pp. 1848-1857.

[3] Miguel Sofo Haro, et al. "Soft X-rays spectroscopy with a commercial CMOS image sensor at room temperature." *Radiation Physics and Chemistry*, Vol. 167, 2020, 108354.

#C17: Atomic and molecular spectroscopy, photo-induced processes

Liquid-jet Velocity Map Imaging

Qi Zhou¹; Dominik Stemer¹; Florian Trinter¹; Henrik Haak¹; Uwe Hergenhahn¹; Gerard Meijer¹; Bernd Winter¹; Iain Wilkinson²

¹ Fritz-Haber Institute

² Helmholtz-Zentrum Berlin

Liquid-Jet Photoelectron Spectroscopy (LJ-PES) [1] enables the direct study of the electronic structure of both solute and solvent, and has advanced the chemical analysis in aqueous solutions. The LJ facilitates in-vacuo continuous liquid replacement, and detection of photoelectrons with minimal collisions with evaporating water molecules.

Velocity Map Imaging (VMI) [2] provides optimal photoelectron collection efficiency with a full 4π steradian range, enabling the measurement of photoelectron angular distributions (PADs) in a single image. While VMI is heavily applied to both solid and gaseous phases [3], its intriguing extension to the aqueous phase remains very challenging. Major experimental and technical difficulties include the disturbance of the focusing electric fields by the presence of the dielectric liquid jet, the background resulting from scattering of the photoelectrons with the (aqueous) solution vapor, and the balance between required high electric fields in a high-vapor environment.

We have overcome the most critical technical issues, and have successfully employed our newly developed Liquid-Jet Velocity Map Imaging (LJ-VMI) setup, comprising precisely tunable high-voltage electrodes and a microchannel plate detector. This system offers a broad dynamical energy range, allowing detection of photoelectrons kinetic energies up to approximately 40 eV. Following initial lab-experiments using laser and ultraviolet light sources, we present here our recent LJ-VMI results obtained at the bending-magnet beamline PM3, at the BESSY-II synchrotron-radiation facility. Data are presented for water, aqueous solutions, as well as non-aqueous solution. We report solute and solvent core-level and valence electron binding energies, show associated PADs, and identify the principal effects of a liquid jet in VMI performance. Next steps in our continuous development of LJ-VMI will be discussed, along the perspective for future applications towards near-ionization-threshold phenomena as well as time-resolved photo-induced reactions and electron dynamics in (aqueous) solution.

[1] B. Winter, M. Faubel, *Chem. Rev.*, 106, 4, pp. 1176–1211, (2006)

[2] A. Eppink, D. Parker, *Rev. Sci. Instrum.*, 68(9), pp. 3477–3484, (1997)

[3] D. M. Neumark, *J. Phys. Chem. A*, 127, 4207–4223, (2023)

#C18: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Detection of surface magnetism by x-ray spectroscopy of hollow atoms

Perla Dergham¹; Christophe Prigent¹; Ch. Vikar Ahmad¹; Amelie Brassard¹; Louis Duval²; Emily Lamour¹; Stéphane Macé¹; Sébastien Steydli¹; Elena Maria Tosi¹; Dominique Vernhet¹; Matthias Werl³; Martino Trassinelli¹

¹ Institut des NanoSciences de Paris, CNRS and Sorbonne University

² Institut des NanoSciences de Paris, CNRS and Sorbonne University and Laboratoire Kastler Brossel, CNRS, ENS-PSL, Collège de France, Sorbonne Université

³ Institute of Applied Physics, TU Wien, Vienna, 1040, Austria

We present the evidence of surface magnetism detection using highly charged ions as a probe, and without any external magnetic field application [1]. Based on x-ray spectroscopy, our investigation puts an end to a longstanding controversy from contradictory studies on ion-magnetic surface interaction based on Auger spectroscopy [2,3]. We measured the $n = 2 \rightarrow 1$ transition of excited argon ions (hollow atoms) produced in grazing incidence collisions of an Ar^{17+} ion beam ($E_{\text{kin}} = 170$ keV) with a monocrystalline (110) nickel sample [4]. When increasing the sample temperature, the $n = 2 \rightarrow 1$ x-ray unresolved transitions show an asymmetric broadening to lower energies, indicating a larger electron population of the $n = 2$ level. This agrees with the expected behaviour of a reduction of the Pauli exclusion effect in the $n = 2$ level (like a reduction of the Pauli shielding effect [5]) as a result of a spin alignment loss of the captured electrons caused by the change of magnetic phase (from a ferromagnetic phase at low temperature to a paramagnetic one at higher temperature). A similar behaviour is observed in $n = 3 \rightarrow 2$ x-ray transition for lower charge incoming argon ions. Because of the selective electron capture of the highly charged ions already above the surface, these findings open new interesting perspectives for the magnetic order surface characterization of the very first atomic layer of samples and of 2D magnetic materials.

[1] P. Dergham, C. Prigent, C.V. Ahmad *et al.*, in preparation for *Phys. Rev. Lett.*

[2] M. Unipan, A. Robin, R. Morgenstern and R. Hoekstra, *Phys. Rev. Lett.* **96** 177601 (2006)

[3] M. Busch, S. Wethekam and H. Winter, *Phys. Rev. A* **78** 010901 (2008)

[4] P. Dergham, F. Aumayr, E. Lamour *et al.*, *Atoms* **10**, 151 (2022)

[5] I. Madesis, A. Laoutaris, T.J.M. Zouros *et al.*, *Phys. Rev. Lett.* **124** 113401 (2020)

#C19: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Theoretical investigation on positron binding properties in water clusters

Daisuke Yoshida¹; Yukiumi Kita²; Tomomi Shimazaki²; Toshiyuki Takayanagi³; Masanori Tachikawa⁴

¹ Tohoku University, Japan

² Yokohama City University, Japan

³ Saitama University, Japan

⁴ Yokohama City University

Positrons, antiparticles of electrons, have been used as versatile diagnostic tools for characterizations of a wide range of materials. In bulk systems, positrons are trapped by open-volume defects and annihilate with electrons, emitting gamma rays, which allows the non-invasive characterization of materials [1]. By recent advances in experimental techniques, positron-molecule bound states and their lifetimes have been observed for various molecules [2]. Furthermore, the potential use of positrons as probes for molecular conformations was predicted by theoretical studies [3].

In this study, we present theoretical investigations of the positron binding and annihilation properties of water clusters of various sizes using the first-principles calculation. Interactions of positrons with atoms and molecules are often compared and contrasted with those of electrons. In water cluster anions, binding energies of the excess electrons are known to exhibit the specific size dependence and distinct binding properties represented by surface- and interior- bound states. For positron-water complexes, while a water monomer cannot bind a positron, while we revealed that a hydrogen bonded dimer can form an electronically stable positron bound state [4]. The polarization effects induced by the hydrogen bond play a crucial role in enhancing the positron binding abilities of the hydrogen bonded binary molecular clusters. Furthermore, we have also investigated positron-water cluster complexes across a wide range of cluster sizes, and identified surface-localized, internally localized, and strongly delocalized binding features, reflecting the structural characteristics of the hydrogen bond networks. We will present the properties of these positronic complexes, highlighting their dependence on cluster sizes, conformers, and the underlying positron binding mechanisms.

References

- [1] F. Tsuomist and I. Makkonen, *Rev. Mod. Phys.* **85**, 1583 (2013).
- [2] G. F. Gribakin, J. A. Young, and C. M. Surko, *Rev. Mod. Phys.* **82**, 2557 (2010).
- [3] A. Swann and G. F. Gribakin: *J. Chem. Phys.* **153**, 184311 (2020).
- [4] D. Yoshida, Y. Kita, T. Shimazaki, and M. Tachikawa, *Phys. Chem. Chem. Phys.* **24**, 26898 (2022).

#C20: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Energy loss function of samarium determined from the reflection electron energy loss spec-troscopy spectra

A. Sulyok¹; Karoly Tokesi²; L.H. Yang³; M. Menyhárd¹; R.G. Zeng⁴; T.F. Yang³; Z.J. Ding⁵

¹ HUN-REN Research Institute for Technical Physics and Materials Science, Centre for Energy Research, ELKH, P.O. Box 49, H-1525 Budapest, Hungary

² HUN-REN Institute for Nuclear Research

³ Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

⁴ National Key Laboratory on Surface Physics and Chemistry, Institute of Materials, China Academy of Engineering Physics, P.O. Box 9071, Jiangyou, Sichuan 621907, People's Republic of China

⁵ Department of Physics, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China and Hefei National Research Center for Physical Sciences at the Microscale, University of Science and Technology of China, Hefei, Anhui 230026, People's Republic of China

Lanthanides have nowadays become of vital importance in advanced materials and technology. Applications in laser science, solar cells, fluorescent lamps and a new organic light-emitting di-odes components, as well as luminescent probes are strongly related with their optical and/or elec-tronic properties.

Samarium and its compounds are among the most frequently used lanthanides in the investigations during the last years. But the precise excitation property, especially the plasmon structure of samarium is still not known. It is not surprising because all lanthanides are highly reactive elements and interact strongly with oxygen and hydrogen. So, experimentally it is really a challenging to obtain accurate results. Da et al. [1] developed a reverse Monte Carlo (RMC) method for the derivation of the energy loss function (ELF) and thereby the dielectric function and optical constants of solids in a much wider photon energy range than that of the usual optical measurements.

Our RMC technique was used to obtain the electron energy loss features buried in the REELS spectra of samarium [2]. The accuracy of the ELF was checked by applying sum rules. We found that the ps-and f-sum rules fulfils very accurately and reach the nominal values with 0.2% and 2.5% accuracy, respectively. We were able to separate the contribution from the bulk and the surface excitations. We show the detailed excitation characteristic in the optical data in the energy range between 3 and 60 eV.

This work was supported by Fund for Bilateral Relationships Between China and Hungary in Science and Technology (S&T) (2021-1.2.4-TÉT-2021-00055).

References

- [1] B. Da B et al., *Journal of Applied Physics*, **113**, 214303 (2013)
- [2] T.F. Yang et al., *Scientific Reports* **13**:3909 (2023)

#C21: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Tailoring optical response of atomic systems with low-dimensional nanoantennas

Karolina Slowik¹; Abhishek Ghosh²; Andres Ayuela³; Antton Babaze⁴; Carsten Rockstuhl⁵; David Dams⁵; Garnett W. Bryant⁶; Marta Pelc²; Marvin M. Müller⁵; Miriam Kosik²

¹ Nicolaus Copernicus University in Toruń, Poland

² Institute of Physics, Nicolaus Copernicus University in Toruń, Poland

³ Centro de Física de Materiales, San Sebastian, Spain

⁴ University of the Basque Country

⁵ Karlsruhe Institute of Technology, Karlsruhe, Germany

⁶ Joint Quantum Institute, Univ. of Maryland, MD, USA

Low-dimensional material structures—such as polyacetylenes and graphene nanoflakes—can function as tunable photonic nanoantennas, offering powerful means to tailor the optical response of nearby atomic systems. Unlike conventional mesoscopic nanoantennas, nanoflakes support a variety of optical resonances, arising from both single-particle excitations and collective modes [1]. In this work, we explore how the nature of these resonances influences the optical response of proximate atomic emitters [2].

Due to the extreme spatial confinement of optical excitations in graphene, effective photonic enhancement demands that the atomic system be placed in close proximity to the nanoflake. At such distances, electron tunnelling between the atom and the nanoantenna becomes possible, introducing a non-negligible electronic back-action that further modifies the nanoflake's optical properties.

We systematically characterize the interplay between optical and electronic couplings and their combined effect on fundamental light-matter interaction phenomena, including coherent coupling and Purcell-enhanced fluorescence. Our analysis uncovers two distinct interaction regimes, determined by the atom-antenna separation, each marked by qualitatively different dynamics [3].

[1] Energy-based plasmonicity index to characterize optical resonances in nanostructures, M.M. Müller, et al., *The Journal of Physical Chemistry C* 124 (44), 24331–24343 (2020)

[2] A. Ghosh et al., in preparation

[3] Revising quantum optical phenomena in adatoms coupled to graphene nanoantennas, M. Kosik et al., *Nanophotonics* 11 (14), 3281–3298 (2022)

#C22: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly

Long-Term Electrostatic Trapping of Multiply Charged Helium Nanodroplets in a Multi-Reflectron Time-of-Flight Device

Matthias Veternik¹; Fabio Zappa²; Paul Scheier²; Elisabeth Gruber²

¹ Institute for Ion Physics and Applied Physics, University of Innsbruck

² Universität Innsbruck

A Multi-Reflectron Time-of-Flight (MR-ToF) device, originally developed through a collaboration between the TU Darmstadt and the University of Greifswald [1], has been adapted to trap multiply charged helium nanodroplets (HNDs) using purely electrostatic fields. The system enables confinement of the droplets for a mean lifetime of about

14 seconds, with individual droplets surviving for over a minute. Successful proof-of-principle measurements demonstrate efficient storage over thousands of revolutions. The achievable storage time is highly sensitive to the vacuum conditions and has been thoroughly characterized as a function of chamber pressure.

The multi-reflectron trap setup provides a versatile platform for investigating excitation-induced processes in doped helium nanodroplets, enabling both the study of weak transitions and time-resolved decay dynamics. Recently, Blackbody Infrared Radiative Dissociation (BIRD) experiments were successfully carried out using the devices vacuum chamber as a blackbody radiation source. These measurements revealed a significant reduction in the mean lifetime of the stored droplets when doped with water clusters. Excitation of intermolecular vibrational modes in the embedded clusters and subsequent heat transfer to the surrounding droplet leads to enhanced helium evaporation, eventually rendering the droplets undetectable as their kinetic energy falls below the detection threshold.

Additional plans for future developments include the integration of a pick-up electrode to monitor changes in charge, mass, and energy of the droplets over time. This implementation will enable novel calorimetric measurements at the nanoscale, providing insights into droplet thermodynamics as well as the possibility for measurements leading to a better understanding of the dynamics of pristine helium droplets, inspired by the work of Hanozin et al. [2], who observed significant charge loss and Rayleigh decay in aqueous droplets.

This research was funded in whole or in part by the Austrian Science Fund (FWF) [10.55776/I6221, 10.55776/V1035].

[1] Schlaich, M.; Fischer, J.; Fischer, P.; Klink, C.; Obertelli, A.; Schmidt, A.; Schweikhard, L.; Wienholtz, F. A Multi-Reflection Time-of-Flight Mass Spectrometer for the Offline Ion Source of the PUMA Experiment. *Int. J. Mass Spectrom.* 2024, 495, 117166. <https://doi.org/10.1016/j.ijms.2023.117166>.

[2] Hanozin, E.; Harper, C. C.; McPartlan, M. S.; Williams, E. R. Dynamics of Rayleigh Fission Processes in ~100 Nm Charged Aqueous Nanodrops. *ACS Cent. Sci.* 2023, 9 (8), 1611–1622. <https://doi.org/10.1021/acscentsci.3c00323>.

#C23: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Observation of many-body dynamical localization

Yanliang Guo

Universität Innsbruck

Chaos and thermalization are interconnected phenomena that happen everywhere in life and play a crucial role in a wide range of scientific fields. A paradigmatic system that exhibits chaotic dynamics is a rotating pendulum that is periodically kicked, the so-called kicked rotor. Surprisingly, for its quantum variant, known as the quantum kicked rotor (QKR), quantum coherence prevents energy absorption, leading to dynamical localization (DL), which can be understood as Anderson localization in momentum space. However, it has been unclear what would happen in presence of interparticle interactions. Here, I report on the experimental observation of many-body dynamical localization (MBDL). We observe this phenomenon with a 1D strongly interacting quantum gas that is subject to a periodic drive. Starting from 2-nK samples in a compensated flat-bottom optical trap, we observe DL in a 1D QKR setting [1] as the interactions are tuned from zero to infinity, i.e., into the Tonks-Girardeau (TG) regime. After some initial evolution, the momentum distribution freezes and retains its characteristic structure as the sample is kicked periodically hundreds of times. In contrast, for random kicking, the distribution becomes uniform and loses all structure, indicating thermalization of the system, irrespective of the interaction strength. Our results give strong evidence for the fact that MBDL is the result of quantum coherence that is maintained in a 1D integrable setting.

[1] Observation of many-body dynamical localization,
Y. Guo et al., arXiv:2312.13880 (2023)

#C24: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Thermal fading of the $1/k^4$ -tail of the momentum distribution induced by the hole anomaly

Giulia De Rosi¹; Grigori E. Astrakharchik¹; Maxim Olshanii²; Jordi Boronat³

¹ UPC - Universitat Politècnica de Catalunya

² University of Massachusetts Boston

³ Departament de Física, Universitat Politècnica de Catalunya

We study the thermal behavior of correlations in a one-dimensional Bose gas with tunable interaction strength, crossing from weakly-repulsive to Tonks-Girardeau regime [1-2]. A reference temperature in this system is that of the hole anomaly [3], observed as a peak in the specific heat and a maximum in the chemical potential. At the anomaly temperature, the spectral states located below the hole branch are thermally occupied and the breakdown of the quasi-particle description occurs. We find that at large momenta k and temperature above the anomaly threshold, the tail C/k^4 of the momentum distribution (proportional to the Tan contact C) is screened by the $1/|k|^3$ -term due to a dramatic thermal increase of the internal energy emerging from the thermal occupation of spectral excitation states. The same fading is consistently revealed in the behavior at short distances x of the one-body density matrix (OBDM) where the $|x|^3$ -dependence disappears for temperatures above the anomaly. We obtain a new general analytic tail for the momentum distribution and a minimum k fixing its validity range, both calculated with exact Bethe-Ansatz method and valid in all interaction and thermal regimes, crossing from the quantum to the classical gas limit. Our predictions are confirmed by comparison with ab-initio Path Integral Monte Carlo (PIMC) calculations for the momentum distribution and the OBDM exploring a wide range of interaction strength and temperature. Our results unveil a novel connection between excitations and correlations. We expect them to be of interest to any cold atomic, nuclear, solid-state, electronic and spin system exhibiting an anomaly or a thermal second-order phase transition.

[1] G. De Rosi, R. Rota, G. E. Astrakharchik, and J. Boronat, Correlation properties of a one-dimensional repulsive Bose gas at finite temperature, *New J. Phys.* **25** 043002 (2023)

[2] G. De Rosi, G. E. Astrakharchik, M. Olshanii, and J. Boronat, Thermal fading of the $1/k^4$ -tail of the momentum distribution induced by the hole anomaly, *Phys. Rev. A* **109**, L031302 (2024)

[3] G. De Rosi, R. Rota, G. E. Astrakharchik, and J. Boronat, Hole-induced anomaly in the thermodynamic behavior of a one-dimensional Bose gas, *SciPost Phys.* **13**, 035 (2022)

#C25: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Zero-Point-Energy Driven Isotopic Exchange of the $[\text{H}_3\text{O}]^-$ anion Probed by Mid-Infrared Action Spectroscopy

Dennis Florian Dinu¹; Milan Ončák²; Sven Thorwirth³; Klaus Liedl²; Sandra Brünken⁴; Stephan Schlemmer³; Pavol Jusko⁵

¹ TU Wien

² University of Innsbruck

³ University of Cologne

⁴ FELIX Laboratory Radboud University

⁵ Max Planck Institute for Extraterrestrial Physics, Garching

We present the first observation of vibrational transitions in the $[\text{H}_3\text{O}]^-$ anion, an intermediate in the anion-molecule reaction of water, H_2O , and hydride, H^- , using a laser-induced isotopic H/D exchange reaction action spectroscopy scheme applied to anions. The observed bands are assigned as the fundamental and first overtone of the $\text{H}_2\text{O}-\text{H}$ -vibrational stretching mode, based on anharmonic calculations within the vibrational perturbation theory and vibrational configuration interaction. Although the $\text{D}_2\text{O}-\text{D}$ -species has the lowest energy, our experiments confirm the $\text{D}_2\text{O}-\text{H}$ -isotope to be a sink of the H/D exchange reaction. Ab initio calculations corroborate that the formation of $\text{D}_2\text{O}-\text{H}$ is favored, as the zero-point-energy difference is larger between D2 and H2 than between $\text{D}_2\text{O}-\text{H}$ and $\text{D}_2\text{O}-\text{D}$.

J. Am. Chem. Soc. 2024, 146, 31, 21634–21641

#C26: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Laser cooling Rydberg molecules - He2

Lucía Verdegay Fernández¹; Bingcheng Zeng¹; Daniel Y. Knapp¹; Jack C. Roth²; Maximilian Beyer¹

¹ VU Amsterdam

² Berkeley University

The helium dimer in its metastable triplet state is a promising candidate to become the first homonuclear molecule ever laser-cooled. Nearly diagonal Franck-Condon factors are obtained, because the electron employed for optical cycling occupies a Rydberg orbital that doesn't take part in the chemical bond. In addition, the general Pauli principle facilitates the closing of the cooling cycle for the rotational degree-of-freedom.

Laser cooling and trapping of the helium dimer would result in a controllable, simple 4-electron system at record low temperature, allowing quantum sensing and precision measurements to test quantum electrodynamics and the quantum nature of collisions with unprecedented accuracy - while being accessible to highly accurate ab initio computational methods.

The prospects for laser cooling He2 are discussed and the rovibronic level structure and transition moments in He2 are analyzed to identify the most suitable electronic transitions for laser cooling. By evaluating the number of scattered photons and the scattering force under different repumping schemes, we determine the optimal optical cycling strategies. Loss mechanisms such as spin-forbidden transitions, predissociation, and ionization processes are studied and found not to introduce significant challenges for cooling.

#C27: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Sunlight and the single atom - a photodetector for fundamental physics and daylight communications

Laura Zarraoa; Morgan Mitchell; Romain Veyron; Tomas Lamich

ICFO - Institute of Photonic Sciences

Emerging photo-detection applications, including ‘light-shining-through-walls’ experiments to search for new particles and interplanetary optical communications, require photodetection with extremely low dark counts and strong background rejection. Here background rejection means filtering to prevent unwanted light (back-ground light) from reaching the photon counting devices. For many contemporary applications, background light comes mainly from the sun: either directly because the photodetector is exposed to sunlight, or indirectly as in the photodetector does not look directly at the sun but is exposed to skylight, which is sunlight scattered from Earth’s atmosphere. In [1], we demonstrated a narrowband quantum jump photodetector (QJPD) to detect single-photons based on a single cold atom and quantified its experimental quantum efficiency and dark count rate. Here, we present the performance of the QJPD in the presence of strong broadband background [2].

The photon counting capabilities of the QJPD under direct and indirect broadband excitation are tested, by measuring quantum jump rates when the atom is illuminated with direct sunlight, and with light scattered by the atmosphere (skylight). A rate equation model is developed to describe QJ probabilities in the presence of both intense broadband background and weak resonant probe light. This model is used to interpret experiments in which a weak signal beam competes with strong broadband background and validated using sunlight, demonstrating a reliable method to extract probe photon numbers even in the presence of background. Measurements where the atom is illuminated with skylight show no observable background-induced QJs.

#C28: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Ab initio simulation of the interplay between an impurity and a measuring environment using ultracold atoms

Katja Schneeweiss¹; Maximilian P. E. Lock²; Tom Rivlin²; Marcus Huber²; Iva Brezinova¹

¹ Institute of Theoretical Physics, Vienna University of Technology

² Atominstitut, Vienna University of Technology

The act of a quantum measurement seems to evade the accessibility of the Schrödinger equation and its unitary time evolution [1]. In this work, we explore whether a quantum measurement on a subsystem by an apparatus can be simulated within an experimentally realizable quantum mechanical many-body system by the unitary time evolution of the many-body Schrödinger equation.

For the numerical simulation, we consider a model inspired by the Fermi-Hubbard model, which is realizable experimentally with ultracold atoms [2] containing a fixed number of indistinguishable fermionic environmental particles and a single distinguishable impurity. The impurity is assumed to be initially in a spatial superposition

but not entangled with the state of the environment. A key advantage of this system lies in the high tunability of its parameters, both experimentally and in simulations.

To simulate the process of a measurement within the many-body Schrödinger equation, the environmental particles are assumed to act as both a measuring apparatus on the impurity and as the environment in a more conventional sense. We determine the exact quantum mechanical time evolution by exact diagonalization of mesoscopically sized systems. We calculate decoherence times and correlation functions for different system sizes, and we study the reduced-density matrix of the impurity and the surrounding environmental particles. We investigate how the spectral properties of the system determine whether the interaction between the impurity and the environment performs a measurement on the impurity or whether the interaction leads to thermalization [3]. To analyze this, the spectral distribution of the eigenvalues of the entire system is calculated as a measure of quantum chaos [4]. The key aim is to identify which degrees of freedom of the surrounding particles act as the measuring apparatus—thereby encoding information about the state of the impurity—and which act as the environment, inducing decoherence.

References:

- [1] Emanuel Schwarzhans, Felix C Binder, Marcus Huber, and Maximilian PE Lock. Quantum measurements and equilibration: the emergence of objective reality via entropy maximisation. *arXiv preprint arXiv:2302.11253*, 2023.
- [2] Immanuel Bloch. Ultracold quantum gases in optical lattices. *Nature physics*, 1(1):23–30, 2005.
- [3] Armando Relano. Decoherence framework for wigner’s-friend experiments. *Physical Review A*, 101(3):032107, 2020.
- [4] Mahdi Kourehpaz, Stefan Donsa, Fabian Lackner, Joachim Burgdörfer, and Iva Brezinova. Canonical density matrices from eigenstates of mixed systems. *Entropy*, 24(12):1740, 2022.

#C29: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Zeeman-Sisyphus deceleration of ultra-cold CaF molecules

Archie Baldock

Durham University

Since the first demonstration of direct laser cooling of molecules, an ever-expanding set of molecular species are being investigated including heavier molecules, polyatomic molecules and “chemically interesting” molecules. While making fast beams of complex and interesting molecules is becoming routine, slowing them to rest such that they can be trapped remains a significant challenge.

Direct laser slowing has been successfully implemented for a select subset of molecules. However, the 10^4 photons required to bring the molecular beam to rest makes it impractical for many species. These species include those with unfavourable branching ratios and heavier molecules which require an even greater number of scattered photons. Zeeman-Sisyphus deceleration presents a novel way to address both concerns. Molecules travel through a spatially varying magnetic field and are optically pumped between high and low field seeking states, meaning they continually climb a potential hill. The optical pumping requires at least two orders of magnitude fewer photons to be scattered compared to direct laser slowing.

The technique has previously been demonstrated for CaOH [1] and YbOH [2], in a two-stage decelerator made up of cryogenic superconducting solenoids. Here, we present our progress in building upon this work to experimentally realise a Zeeman-Sisyphus decelerator for CaF. Our implementation follows [3], using 80 stages of permanent magnets at ambient temperatures.

- [1] B.L. Augenbraun, et al, Phys. Rev. Lett. 127, 263002 (2021)
 [2] H. Sawaoka, et al, Phys. Rev. A 107, 022810 (2023)
 [3] N.J. Fitch, and M. R. Tarbutt, ChemPhysChem 17, 22 (2016)

#C30: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Efficient loading of ultracold atoms into standing wave potential near dielectric surface

Ryota Hashimoto¹; Hayato Kawamura²; Taro Mashimo¹; Satoshi Tojo³

¹ Department of Physics, Chuo University,

² Department of Physics, Chuo University

³ Department of Physics, Chuo University

Abstract

Precise manipulation of ultracold atoms is one of powerful methods for investigation of complicated fields as a quantum sensor. We have investigated interactions between a dielectric surface and atoms [1, 2], and manipulation of cold atoms by optical dipole and radiative forces [3].

In this study, we have experimentally observed the loading behaviors of ultracold rubidium atoms into the dielectric surface region. The pre-cold atoms are loaded into an optical dipole trap and vertically transported to dielectric surface region by controlling the focus position of the trapping beam with a motorized stage. In the surface region, the trapping beam is reflected and forms standing waves.

We have experimentally observed the effective loading ultracold atoms with a temperature of $10\mu\text{K}$ into the standing wave potential which suppresses the atom loss and the oscillation behavior. These results indicate initially trapped atom in the standing wave with high phase-space-density condition and lead into Bose-Einstein condensate in the vicinity of the dielectric surface.

References

- [1] Athanasios Laliotis, Bing-Sui Lu, Martial Ducloy, and David Wilkowski, AVS Quantum Sci. 3 043501 (2021).
 [2] Kosuke Shibata, Satoshi Tojo, and Daniel Bloch, Optics Express 25 9476 (2017).
 [3] Taro Mashimo, Masashi Abe, and Satoshi Tojo. Phys. Rev. A 100, 063426 (2019).

#C31: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Josephson Oscillations in long ballistic channels

Simon Wili¹; Mohsen Talebi²; Tommaso Bonaccorsi¹; Michael Mühlematter¹; Yaakov Yudkin¹; Meng-Zi Huang¹; Tilman Esslinger¹

¹ ETH Zürich

² ETH

Josephson Oscillations (JO) have been studied in cold atom experiments with Bose-Einstein condensates and strongly interacting Fermi gases, where they typically occur across a thin tunneling barrier. In this work, we present measurements of JO occurring between two reservoirs containing unitary Fermi gases. The reservoirs are connected by a long, mesoscopic transport channel projected by a

digital micromirror device. We vary the size and geometry of the channel as well as the reservoirs' temperatures to explore the robustness of the JO.

#C32: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Cryogenic apparatus for quantum logic spectroscopy of polyatomic molecular ions

Mikhail Popov; Nanditha Sunil Kumar; Prerna Paliwal; Stefan Willitsch

University of Basel

Due to the complexity of their internal energy level structure, controlling molecules' internal states presents a significant challenge. Most molecular ions lack closed optical cycling transitions, which prevents standard state preparation and detection techniques routinely exploited in the atomic community, as well as direct laser cooling techniques. These challenges were recently tackled for some diatomic molecules employing quantum logic spectroscopy techniques (QLS) [1-3]. Unlike diatomic species, polyatomic ones exhibit new properties such as isomerism, chirality, and parity doublet states, which may be employed in tests of fundamental physical theories [4].

We aim to extend QLS methods to polyatomic molecular ions. Our approach involves the state preparation of molecular ions using a resonant-enhanced multiphoton photoionization technique [5]. The state-prepared molecular ion is trapped and sympathetically cooled inside a crystal of laser-cooled Ca ions. The state of the molecular ion is then detected using a single co-trapped Ca ion by exerting a state-dependent off-resonant optical dipole force on the molecule and reading out the resulting motional excitation of the ion crystal.

Here we discuss the progress in the construction and initial characterization of a cryogenic ion trapping setup, which will be used for trapping and QLS of polyatomic molecular ions, as well as for cold chemistry and collision studies on a state-to-state level.

- [1] M. Sinal, Z. Meir, K. Najafian, G. Hegi, S. Willitsch, Science 2020, 367(6483), 1213.
 [2] F. Wolf, Y. Wan, J. C. Heip, F. Gebert, C. Shi, P. O. Schmidt, Nature 2016, 530(7591), 457-460.
 [3] C. W. Chou, C. Kurz, D. B. Hume, P. N. Plessow, D. R. Leibbrandt, D. Leibfried, Nature 2017, 545(7653), 203-207.
 [4] L. Anderegg, N. B. Vilas, C. Hallas, P. Robichaud, A. Jadbabaie, J. M. Doyle, N. R. Hutzler, Science 2023, 382(6671), 665-668.
 [5] X. Tong, A. H. Winney, S. Willitsch, Physical Review Letters 2010, 105(14), 143001.

#C33: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Universal momentum tail of identical one-dimensional anyons with two-body interactions

Raúl Hidalgo Sacoto¹; D. Blume²; Thomas Busch¹

¹ Quantum Systems Unit, Okinawa Institute of Science and Technology Graduate University

² Homer L. Dodge Department of Physics and Astronomy, The University of Oklahoma

Non-relativistic anyons in 1D possess generalized exchange statistics in which the exchange of two identical anyons generates a non-local phase that is governed by the spatial ordering of the particles and the statistical parameter α . Working in the continuum, we demonstrate the existence of two distinct types of 1D anyons, namely bosonic anyons and fermionic anyons. We identify a many-body Hamiltonian with additive two-body zero-range interactions that supports bosonic and fermionic anyon eigenstates, which are, for arbitrary interaction strength, related through a generalized bosonic-anyon—fermionic-anyon mapping, an extension of the celebrated Bose-Fermi mapping for zero-range interacting 1D systems. The momentum distributions of bosonic and fermionic anyons are distinct: while both feature k^{-2} and k^{-3} tails, the associated prefactors differ. Our work reveals intricate connections between the generalized exchange statistics, the universal two- and three-body Tan contacts of systems consisting of N identical particles, and the emergence of statistics-induced chiral symmetry breaking.

#C34: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Topological transport properties of height modulated subwavelength barrier lattices

Giedrius Žlabys¹; Wen-Bin He¹; Sarika Sasidharan Nair¹; Thomas Busch²; Tomoki Ozawa³

¹ Okinawa Institute of Science and Technology Graduate University

² OIST Graduate University

³ Tohoku University Advanced Institute for Materials Research

Ultracold atom gases trapped in optical potentials offer a clean and controllable platform to realize quantum models that are difficult to implement in condensed matter systems [1]. Recent theoretical [2] and experimental [3] developments allow to create periodic sub-wavelength potentials that overcome the diffraction limit imposed by the wavelength of the used laser beams. These potentials support the paradigmatic Kronig-Penney-type models which not only describe the behavior of electrons in a one-dimensional crystal but also have been shown to host topologically protected edge states [4]. Developing control strategies for such systems is of fundamental interest in quantum technologies that rely on robust states for computations [5].

In this work we analyze the topological properties of an advanced Kronig-Penney model. The emergent topological behavior is observed under translations and height modulation of the periodic potential in one dimension. The energy bands split into sub-bands displaying Hofstadter's butterfly-like structure under the change of the spatial modulation frequency. This leads to the redistribution of the topological invariants classifying the bands to a set of sub-bands indicating the same charge transport at lower filling. The transport is realized via adiabatic pumping and the spectral function is calculated showing the existence of topologically protected flat edge modes in the many-body

case [6,7].

[1] P. Windpassinger et al., Rep. Prog. Phys. **76**, 086401, (2013)

[2] M. Lacki et al., Phys. Rev. Lett. **117**, 233001, (2016)

[3] Y. Wang et al., Phys. Rev. Lett. **120**, 083601, (2018)

[4] I. Reshodko et al., New J. Phys. **21**, 013010, (2019)

[5] C. P. Koch et al., EPJ Quantum Technol. **9**, 1, (2022)

[6] W.-B. He et al., Phys. Rev. A **111**, 013312, (2025)

[7] S. S. Nair et al., Phys. Rev. A **111**, 033313, (2025)

#C35: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Light-Induced Losses and Pauli Suppression of Inelastic Collisions in a Sample of Trapped Bosonic Feshbach Molecules of $^{161}\text{Dy}^{40}\text{K}$

Luc Absil¹; Alberto Canali²; Chun Kit Wong²; Marian Kreyer²; Emil Kirilov³; Rudolf Grimm²

¹ Institut für Experimentalphysik, Universität Innsbruck

² Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria

³ Institut für Quantenoptik und Quanteninformation (IQOQI), Österreichische Akademie der Wissenschaften, Innsbruck, Austria. Institut für Experimentalphysik, Universität Innsbruck, Austria

We have studied the loss mechanisms in a sample of trapped ultracold bosonic Feshbach molecules formed from the fermionic isotopes ^{161}Dy and ^{40}K . Created by sweeping a magnetic field across a low-field Feshbach resonance at 7.29 G [1], the sample consists of approximately 7000 molecules at a typical temperature of 70 nK. The molecules are spatially separated from the remaining atomic cloud using a Stern-Gerlach technique while being held in an optical trap [2].

By measuring the lifetime of the molecules primarily in a 1064 nm optical dipole trap, we identified a dominant one-body loss contribution, proportional to the intensity of the trapping light and the closed-channel fraction of the Feshbach molecules. This suggests a one-photon coupling to electronically higher excited states of the molecular manifold. We therefore performed loss spectroscopy measurements at four different wavelengths. The linear dependence of loss rates on intensity was found to increase by two orders of magnitude, allowing us to isolate the two-body losses in the 1547 and 2002 nm traps.

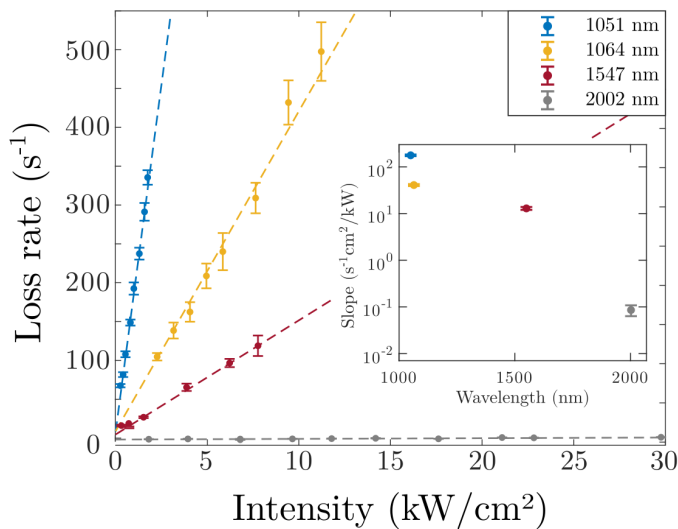
We were then able to demonstrate Pauli suppression of collisional losses by a factor of four in the 1547 nm trap. At 2002 nm, despite a measured lifetime of 400 ms at 60 mG from the resonance, technical limitations prevented us to get closer from the resonance.

These results pave the way toward the realization of quantum-degenerate DyK molecules and exotic superfluid states derived from our mass-imbalanced fermion mixture.

Fig.: Linear dependence of the measured one-body loss rates on the intensity of the single-beam trapping light at four different wavelengths.

[1] Z.-X. Ye, et al., Phys. Rev. A **106**, 043314 (2022).

[2] E. Soave, et al., Phys. Rev. Res. **5**, 033117 (2023).



#C36: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Interfacing Rydberg atoms with a high overtone bulk acoustic wave resonator in the GHz regime

Julia Gamper; Cedric Wind; Valerie Mauth; Samuel Germer; Wolfgang Alt; Sebastian Hofferberth

Bonn University

Rydberg atoms exhibit strong electric dipole transitions over a large range of the electromagnetic spectrum, making them ideal candidates for hybrid quantum systems that connect the optical and microwave domains.

In this project, we plan to investigate the coupling between optically controlled Rydberg atoms and a high overtone bulk acoustic wave resonator (HBAR). Our goal is to explore the potential to cool and control one of the resonator's acoustic modes to its quantum mechanical ground state by exchanging microwave photons with the Rydberg atoms.

This poster presents our approach to realize such a hybrid system. We describe the design and construction progress of our setup with our solution for the initial laser cooling of rubidium atoms and their transport to the cryogenic environment. To couple Rydberg atoms to the HBAR, it is necessary to bring the atoms close to the resonator surface. For this purpose, we plan to implement an on-chip magnetic trap. In a first generation, this chip will contain an integrated microwave resonator instead of the HBAR to test the individual steps such as atom trapping, Rydberg excitation and electric field control. The next-generation atom chip will include the HBAR to enable the planned experiments.

#C37: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Towards all-optical entangled BECs in microgravity

Jan Simon Haase¹; Viviane Wienzek¹; Alexander Fieguth²; Igor Bröckel²; Jens Kruse²; Carsten Klempt³; INTENTAS Colaboration⁴

¹ Institut für Quantenoptik, Leibniz Universität Hannover

² Deutsches Zentrum für Luft- und Raumfahrt SI

³ Deutsches Zentrum für Luft- und Raumfahrt SI; Institut für Quantenoptik, Leibniz Universität Hannover

⁴ Humboldt Universität zu Berlin; Deutsches Zentrum für Luft- und Raumfahrt SI; Technische Universität Darmstadt, Fachbereich Physik, Institut für Angewandte Physik; Institut für Quantenoptik, Leibniz Universität Hannover; Ferdinand-Braun-Institut Berlin; Leibniz Universität Hannover, Institut für Transport- und Automatisierungstechnik; Institut für Quantenphysik und Center for Integrated Quantum Science and Technology (IQST), Universität Ulm

Atom interferometers are high-precision sensors for acceleration, rotation and magnetic fields. Space-borne atom interferometers promise a wide range of applications from geodesy to fundamental tests of physics. Their improved sensitivity due to prolonged interrogation times benefits from the macroscopic coherence length and slow expansion rates of Bose-Einstein condensates (BECs). A limit for the precision is the Standard Quantum Limit. By using entangled ensembles of atoms, the limit can be surpassed, improving the sensitivity of interferometric measurements.

The INTENTAS project is designed as a source of entangled atoms that can be operated on a microgravity platform. To demonstrate sensitivity beyond the Standard Quantum Limit, a rubidium BEC is generated, entangled via spin-changing collisions and detected with high resolution. For the generation process a fast, compact and robust system is necessary. Here, an all-optical approach has been chosen in order to avoid any structure, conducting surface or magnetic field located in the vicinity of the atoms. Using this a 2 Hz repetition rate has been achieved in a dedicated lab experiment. Furthermore, INTENTAS explored the capabilities of arbitrary shaped potentials via time-averaged potentials deployed in the all-optical approach. In this contribution I will present an overview of the experimental setup, measurement results from ground operation and insights from operation in the Einstein Elevator, a high repetition microgravity platform.

#C38: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Tunable Field-Linked s-Wave Interactions in Dipolar Fermi Mixtures

Jinglun Li¹; Georgios M. Koutentakis¹; Mateja Hrast¹; Mikhail Lemeshko¹; Andreas Schindewolf²; Ragheed Alhyder¹

¹ Institute of Science and Technology Austria (ISTA)

² Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien

Spin mixtures of ultracold fermions are a cornerstone of quantum many-body physics, enabling superfluidity, polaron formation, and rich spin dynamics. Introducing strong, long-range dipolar forces into such mixtures promises even more exotic phases, but has been hampered by the loss of two molecules at short range. Microwave dressing can prevent the gas from the short-range collapse and induce the

field-linked scattering resonance. This shield has already stabilised the first shallowly degenerate gas of dipolar fermions, but only with a single internal state, leaving the physics of spin mixtures largely unexplored. Here, we show that introducing a second spin state unlocks a new and simple handle on interactions. In particular, tuning the microwave power sweeps the s-wave interaction from strongly attractive to strongly repulsive, crossing a field-link scattering resonance. This control enables fast s-wave evaporative cooling and opens new routes to stable, strongly interacting dipolar Fermi gases.

#C39: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Bosons in a 1D Quasiperiodic Optical Lattice studied via tVMC method

Nikola Vukman¹; Mathias Gartner²; Ferran Mazzanti³; Petar Stipanovic¹; Leandra Vranjes Markic¹; Robert Zillich²

¹ Faculty of Science, University of Split, Split, Croatia

² Institute for Theoretical Physics, Johannes Kepler University, Linz, Austria

³ Departament de Física i Enginyeria Nuclear, Universitat Politècnica de Catalunya, Barcelona, Spain

A systematic study of bosons in a one-dimensional quasiperiodic optical lattice is performed using the Quantum Monte Carlo time-dependent Variational Monte Carlo (tVMC) method [1], following the procedures established by some of the authors in an earlier study [2]. In quasiperiodic lattices, formed by the superposition of two optical lattices with incommensurate wave numbers, even a weak secondary lattice is known to induce localization in non-interacting systems [3, 4]. The present work investigates the delocalization effect of two-body contact interactions. Ground state observables, such as the density profile and pair distribution function $g_2(r)$, are obtained via imaginary-time evolution for different quasiperiodic lattice configurations, where the relative strength of the secondary lattice is varied and both shallow and deep primary lattices are considered. A weak perturbation pulse is then applied within the linear response regime to study the system's dynamical behaviour via real-time evolution, characterized by the dynamic structure factor $S(k, \omega)$. Comparison with selected results from periodic optical lattices [2], as well as a broader analysis spanning from the weakly interacting regime to the strongly interacting limit, is performed. The tVMC method enables the exploration of regimes beyond mean-field-like and Hubbard model approximations. The results reveal the emergence of rich structural and dynamical phenomena in quasiperiodic lattices compared to their periodic counterparts.

References:

- [1] G. Carleo et al., Phys. Rev. A 89, 031602 (2014).
- [2] M. Gartner et al., SciPost Phys. 13, 025 (2022).
- [3] P. W. Anderson, Phys. Rev. 109, 1492 (1958).
- [4] E. H. Lieb and W. Liniger, Phys. Rev. 130, 1605 (1963).

#C40: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Construction and Characterization of a Ca Magneto-Optical Trap for Rydberg Physics

J. A. L. Grondin; E. Marin-Bujedo; Th. Schiltz; Th. Corbo; Matthieu G  n  vriez

Universit   catholique de Louvain

Ultracold gases of divalent atoms excited to high Rydberg states are an exciting tool to explore subjects from fundamental Rydberg physics to quantum simulation [1]. While calcium has received little attention compared to other heavier divalent species (Sr, Yb), its unique features, including low autoionization rates or the smallest electronic affinity of all atomic species, are expected to open up new possibilities to control, manipulate and study Rydberg gases. We will report on the development of an experimental setup for ultracold calcium Rydberg atoms.

Our experimental setup features a custom-made oven combined to a 3D-printed permanent-magnet Zeeman slower, for first stage cooling of calcium atomic beam. Atoms exiting the Zeeman slower at velocities near 30 m/s are then trapped in a magneto-optical trap whose magnetic-field gradient is generated by a pair of home-built coils with an original water-cooling scheme. This approach allows us to prepare a trapped ensemble of Ca atoms at a temperature of a few mK. We then employ a resonant three-photon scheme to excite ground-state atoms to $4snp\ ^1P$ and $4snf\ ^1F$ Rydberg states. The measurement of the detailed properties of the calcium trap, together with the modelling and characterization of the Rydberg excitation, is currently under way and will be reported in our communication. With the present setup, we will be in a position to investigate the direct cooling of Rydberg atoms with an isolated core transition [2] or high lying doubly excited "planetary" states of the Ca atom.

[1] Dunning, F. B. et al., J. Phys. B. 49, 112003 (2016).

[2] Bouillon, A. and Marin-Bujedo, E. and G  n  vriez, M., Phys. Rev. Lett. 132, 193402 (2024).

#C41: Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

A cavity-microscope for micrometer-scale control of atom-photon interactions

Francesca Orsi; Rohit Prasad Bhatt; Ekaterina Fedotova; Michael Eichenberger; L  a Dubois; Jean-Philippe Brantut

EPFL

Cavity quantum electrodynamics studies the strong interaction between matter and the electromagnetic field of an optical cavity: the enhanced interaction is useful both for reading the properties of the atoms with a fast, sensitive and weakly destructive measurement and for quantum simulation where atoms interact by exchanging photons with each other at a distance. One of the drawbacks of these systems is the loss of spatial information that cavity-based measurement implies: the result of these measurements is an average of the properties of the atoms over the entire cavity field volume.

I will explain how we built and operated a cavity-microscope device that overcomes this problem: it realizes both a cavity and a pair of high numerical-aperture lenses in a single device and can be used to couple a microscopic part of the atomic cloud to the cavity field. We produce a cavity-based image of the atomic density by scanning the position of the microscope focus [1].

This technology opens the doors to analog quantum simulations of programmable, all-to-all interacting systems. I will report about the self-organization phase transition of a Fermi gas in a high-finesse cavity in the presence of tight confinement and the development of optical techniques to randomize cavity-mediated interactions. These interactions can drastically change the behavior of the system, and open the door to the exploration of models of holographic quantum matter such as the Sachdev-Ye-Kitaev model [2].

#C42: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Single and Double Ionization of Sn^+ and Sn^{2+} by Electron Impact

Mohammad Gharaibeh¹; Alex Borovik²; Alfred Müller²; Károly Tőkési³; Pierre-Michele Hillenbrand²; Stefan Schippers⁴

¹ Qatar University

² Justus-Liebig-Universität Gießen

³ HUN-REN Institute for Nuclear Research (ATOMKI)

⁴ Justus-Liebig-Universität Gießen, 4Helmholtz Forschungsakademie Hessen für FAIR (HFHF)

A systematical investigation of the electron-impact ionization cross sections of Sn^+ and Sn^{2+} ions has been performed by employing a crossed-beams technique. Single- and Double-Ionization cross sections for these ions were measured within energy ranges from the ionization threshold to 1000 eV. The study uncovers contributions from indirect ionization processes, involving the ionization or excitation of inner electron subshells. These insights are valuable for advancing the understanding of electron-ion interactions and supporting plasma modeling efforts, as well as applications in extreme ultraviolet (EUV) lithography. The findings underscore the critical role of accurate experimental data in refining theoretical models for complex atomic systems. Configuration-Averaged Distorted Wave (CADW) direct ionization cross section calculations using the Los Alamos National Laboratory (LANL) were performed for comparison. The Classical Trajectory Monte Carlo (CTMC) method was used to determine the electron impact single ionization cross sections for Sn^+ ; the CTMC simulations were made in the three-body approximation. These two theoretical calculations included the excitations from inner shells as well as the ground state. Both theoretical approaches show qualitative agreement with the total experimental cross-sections.

#C43: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Negative Ion Chemistry Among Stars And Clouds: Molecular Processes In The Interstellar Medium

Franco Gianturco

University of Innsbruck

The last ten years or so have witnessed a tremendous growth on the detection and observation of charged molecular species in the interstellar medium (ISM), especially within the special environments provided by interstellar and circumstellar clouds. Further observations within the atmospheres of the exoplanets have confirmed the marked ubiquity of these most diverse chemical species in the rather hostile

environments of the interstellar space and identified specific regions that are considered to be the most efficient laboratories for molecular formation processes involving molecular anions. In the present talk I shall draw examples from our recent works on the study of molecular mechanisms presiding over ion-molecule reactions which lead to those anionic molecular products which have already been astronomically observed. We have been investigating the most efficient paths which can guide the formation of the recently observed carbon-rich molecular anions and on a variety of possible molecular quantum processes which can take place in the Diffuse and Dark regions of the interstellar clouds and in the atmospheres of some of the exoplanets.

1. F.A. Gianturco et al., Phys. Rev.Lett. 127, 043001 (2021).

2. F.A.G. et al., Phys. Rev. Lett., 131, 183002 (2023).

3. F.A.G. et al., The Astrophys. J. 897, 75-88, (2020)

4. F.A.G. et al., Faraday Disc., 212, 117 (2018).

5. F.A.G. et al., The Astrophys. J., 850, 42 (2017).

6. F.A.G. et al., J. Chem. Phys. 153, 184309 (2020).

7. F.A.G. et al., MNRAS, 522, 5775-5787 (2023).

8. F.A.G. et al., The Astrophys. J., 960, 40-52 (2023).

9. F.A.G. et al., The Astrophys. J., 973, 17 (2024)

#C44: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

The quadrupole ion trap apparatus for ionization cross-section experiments

Mariusz Piwinski¹; Łukasz Kłosowski²

¹ Nicolaus Copernicus University in Toruń

² Nicolaus Copernicus University in Toruń

The electron collision experiments provide essential information on the structure of the bombarded objects. The obtained data on the cross-sections of the studied process are a valuable addition to information obtained using the optical spectroscopy technique. Such data can be found both numerically and experimentally. The measurements usually involve bombarding the selected target with a beam of electrons and detecting the non-scattered electrons (transmission methods) or scattered electrons (crossed beams technique). Cross-fired or cell experiments are relatively simple for the neutral target. The situation becomes more complicated if one considers the electron impact on ions. It is generally difficult to provide a beam of ions of sufficiently well-defined geometry and density, allowing the detection of scattered electrons with good statistics. These are the main reasons for only a few experiments on electron collisions with singly charged ions.

On the other hand, there are several theoretical datasets on calcium ion ionization [1–4]. Moreover, the data on the ionization of ions may be especially interesting, as, besides direct ionization, one can observe autoionizing processes, which play a significant role in the process at specific energies.

An ion trap can be used as a container for target ions to overcome this problem. In this case, the target can be detected instead of the projectile, which can be achieved using optical methods similar to depletion spectroscopy [5]. In electron-atom/ion collision experiments, cross-section data are typically presented as a function of electron energy. Therefore, precise energy control of the monochromatic electron beam is important as it determines the quality of the obtained data. Unfortunately, the RF field used in the trap can disturb both the energy and electron trajectories. Therefore, optimizing the system in this respect is crucial for the quality of the obtained data.

We present a new experimental system using a quadrupole ion trap with an integrated electron gun. In the applied geometry, the electron beam is emitted along the axis of the trap, which reduces the energy spread of electrons and thus increases the accuracy of measurements.

[1] P.G. Burke, A.E. Kingston, A. Thompson, Electron impact ionisation of Ca+, J.Phys. B: At. Mol. Phys. 16 (13) (1983) L385–L389.

[2] D.C. Griffin, M.S. Pindzola, C. Bottcher, Calculations of the contributions of excitation-autoionisation to the electron impact ionisation

of Ca⁺ and Ba⁺ in the distorted-wave approximation, *J. Phys. B: At. Mol. Phys.* 17 (15) (1984) 3183–3191.

[3] M.S. Pindzola, C. Bottcher, D.C. Griffin, Indirect processes in the electron impact ionisation of Ca⁺ using an LS-term-dependent close-coupling method, *J. Phys. B: At. Mol. Phys.* 20 (14) (1987) 3535–3545.
[4] N.R. Badnell, D.C. Griffin, M.S. Pindzola, Electron impact ionization of Ca⁺, *J. Phys. B: At. Mol. Opt. Phys.* 24 (11) (1991) L275

[5] Ł. Kłosowski, M. Piwiński, Experimental method for determination of the integral cross-section for electron impact ionization of ions with optical control of the target's initial quantum state, *J. Electron. Spectrosc. Relat. Vol.* 260, 147239 (2022), p. 1-8

#C45: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electron collisions with molecular hydrogen for plasma-modelling applications

Liam Scarlett¹; Mark Zammit²; Igor Bray¹; Dmitry Fursa¹

¹ Curtin University

² Los Alamos National Laboratory

We present a summary of cross sections for electron scattering on H₂ for fusion and astrophysical plasma-modelling applications, calculated using the molecular convergent close-coupling (MCCC) method. Accurate collisional-radiative modelling requires the input of cross sections for numerous processes, including elastic scattering, ionisation, and excitation, considering a large number of different initial and final states. For molecules, resolution in the vibrational and rotational levels is often required.

Over the last few decades, the CCC method has been established as one of the world's most accurate techniques for calculating collision cross sections, with its particular strength in being able to solve the scattering equations over the entire incident energy range for most processes of practical interest. The application to scattering on molecules with a focus on calculating rovibrationally-resolved cross sections has led to the largest set of collision data ever produced for any scattering system. A dedicated database (mccc-db.org) is established for the data also available from the IAEA database CollisionDB.

In this poster we showcase results for electron collisions with H₂, with examples of applications in fusion and astrophysical plasma models. Comparisons are made with previously available data, wherever available. However, the majority of data we have produced is the first of its kind. The attached figure compares the results of a collisional-radiative (CR) model for the triplet system of H₂ using MCCC cross sections [1] as well as cross sections from two previous datasets [2,3] with measurements [4]. The CR model using MCCC cross sections yields much better agreement with experiment.

[1] L. H. Scarlett et. al., *Atom. Data Nucl. Data Tables* **137**, 101361 (2021)

[2] R. K. Janev et. al., "Collision processes in low-temperature hydrogen plasmas", Jülich (2003)

[3] Miles et. al., *J. Appl. Phys.* **43**, 678 (1972)

[4] Wunderlich et. al., *J. Phys. D: Appl. Phys* **54**, 115201 (2021)

#C46: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Cryogenic hybrid trapping of Ca⁺ ions and OH molecules for cold ion-molecule reaction studies

Yanning Yin; Christian Mangeng; Richard Karl; Pietro Vahramian; Stefan Willitsch

University of Basel

Over the past 15 years, the development of hybrid trapping experiments for cold atoms and ions has enabled a variety of new research directions and applications in the realm of atomic, molecular and chemical physics [1]. We introduce here an extension of this approach to the molecular domain by combining an ion trap and a molecular trap as a new way to explore low-temperature ion-molecule collisions.

We present an experimental realization of a hybrid trap for OH molecules and Ca⁺ ions, with the potential to implement other molecular ions through sympathetic cooling. A supersonic beam of OH radicals is decelerated using a Stark decelerator and loaded into a magnetic trap formed by permanent magnets [2]. The Ca⁺ ions are initially trapped and Doppler cooled in one stage of a segmented linear Paul trap and then transported to be overlapped with the trapped OH molecules.

Once superimposed, strong magnetic field gradients from the OH trap induce position-dependent Zeeman shifts on the Ca⁺ ions disrupting laser cooling. This is mitigated using two cooling lasers with precisely tuned wavelengths and polarizations, along with a repumping laser, enabling efficient cooling to millikelvin temperatures comparable to field-free conditions [3,4].

With the successful realization of the hybrid trap, cold collisions between OH molecules and Ca⁺ ions are being investigated in our lab. First experimental results will be presented, along with a novel method for determining the number and temperature of Coulomb-crystallized ions using convolutional neural networks [5].

[1] M. Deiß, S. Willitsch and J. H. Denschlag, *Nat. Phys.* **20**, 713 (2024)

[2] D. Haas, C. von Planta, T. Kierspel, D. Zhang, and S. Willitsch. *Commun. Phys.* **2**(1), 101 (2019)

[3] R. Karl, Y. Yin, and S. Willitsch. *Mol. Phys.* 2199099 (2023)

[4] C. Mangeng, Y. Yin, R. Karl, and S. Willitsch. *Phys. Rev. Research* **5**(4), 043180 (2023)

[5] Y. Yin, and S. Willitsch. *arXiv:2502.18442* (2025)

#C47: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

The lifetime of a freely decaying hollow atom

Matthias Werl¹; Anna Niggas¹; Filip Vuković¹; Friedrich Aumayr¹; Károly Tőkési²; Richard Wilhelm¹; Sophie Wrathall¹; Victoria Vojtech¹

¹ TU Wien

² HUN-REN Institute for Nuclear Research (ATOMKI)

A highly charged ion (HCI) captures electrons resonantly from a surface upon impact. This capture takes place into highly excited ionic states, leaving intermediate shells empty and creating a hollow atom (HA) [1,2]. The subsequent de-excitation of these HAs can be quite complex and depends strongly on whether it decays freely in vacuum or close to a target surface [3].

In this contribution, experimental results on the de-excitation of HCIs

of various mass, charge states and energies will be presented. It will be discussed how the de-excitation is different in transmission experiments through 2D materials [4] and in grazing incidence scattering geometry from a surface [5]. In grazing incidence scattering it is possible to avoid surface-near processes such as the interatomic coulombic decay, which would otherwise lead to an ultra-fast (fs) de-excitation. We further present a comprehensive model calculation for highly excited HAs and their de-excitation cascade. Our code [5] takes radiative and non-radiative transition rates computed using the flexible atomic code (FAC) [6] as input and we account for screening and mirror charge effects. We find that for a free decay in vacuum the total lifetime of an HA is typically in the picosecond range. Additionally, we could show that under certain conditions, HAs can survive for up to 10 ps. This would make them in principle available for further studies and use in experiments.

[1] J.-P. Briand et al., Nucl. Instrum. Methods Phys. Res., B 154, 166-173 (1999)

[2] J. Burgdörfer et al., Phys. Rev. A 44, 9 (1991)

[3] R.A. Wilhelm et al., Phys. Rev. Lett. 119, 103401 (2017)

[4] A. Niggas et al., Commun. Phys. 4, 180 (2021).

[5] M. Werl et al., Phys. Rev. Res. 7, 013176 (2025)

[6] M.F. Gu, Can. J. Phys., 86, 675 (2008)

#C48: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Measuring ion-induced biomolecular fragmentation using a Velocity Map Imaging spectrometer

Antonin Bourgeteau; Alain Méry; Jimmy Rangama; Jean-Yves Chesnel; Violaine Vizcaino

CIMAP

The study of the interactions between ion beams and biomolecules such as nucleobases, nucleosides, amino acids or peptides is a relevant topic for hadrontherapy applications. After interaction with the energetic ions, the biomolecular target could be ionized and excited. Molecular fragmentation is one of the relaxation process for such ionized/excited states. To better quantify the fragmentation channels and the collision processes, it is interesting to measure the differential cross-sections of the created fragments in both kinetic energy (KE) and emission angle. The kinetic energy of the emitted fragment gives, indeed, information on the electronic state of the transient molecular ions prior dissociation. To do so, a Velocity Map Imaging (VMI) spectrometer initially designed to measure ion-induced electron emission from biologically relevant molecules [1] has been adapted to study fragmentation dynamics.

In the experimental set-up, the pulsed projectile ion beam crossed perpendicularly a continuous target beam produced from an effusive cell. The fragments formed in the interaction volume are velocity focused by a multi-electrode VMI spectrometer onto the 2D position sensitive detector (PSD) mounted after a flight tube. The time-of-flight (ToF) arrival signals are used to distinguish the fragments according to their m/q ratio with m and q , the mass and the charge state of fragment respectively. The detector is pulsed in order to image only a specific m/q specie determined by its ToF. An inverse Abel transform is then performed to the image to reconstruct the initial velocity vector and deduce both kinetic energy spectra and emission angle. The mass resolution of the spectrometer depends, in part, on the flight tube length. We have therefore designed a longer flight tube to improve the resolution, which allows us to access to both the kinetic energy and emission angle for many fragments of complex molecules that we could not separate before.

In this contribution, the new design of the VMI spectrometer will be presented. Moreover, the different fragmentation pathways of Uracil and Adenine upon 120keV-Ar⁸⁺ collision will be discussed based on the KE spectra measured. The influence of the target beam initial velocity on the images of fragments that leave with a low kinetic energy

will also be discussed. Indeed, due to Maxwell-Boltzmann velocity distribution of the target beam, the images are shifted and distorted, presenting a more elliptical shape. A deconvolution method using a Wiener filter has been implemented on the experimental images to remove the influence of the target initial speed with rather satisfactory results.

[1] Nicolas Sens, Michal Ryszka, Jean-Christophe Pouilly, Alain Méry, Jean-Yves Chesnel, and Violaine Vizcaino. A velocity map imaging spectrometer for measuring absolute differential cross sections for ion-induced electron emission from molecules. Rev. Sci. Instrum. 93, 085103 (2022)5

#C49: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electron-Induced Fluorescence of Carbon Monoxide

Enmily Garcia¹; Barbora Stachova¹; Samuel Peter Kovár¹; Peter Papp¹; Dennis Bodewits²; Steven Bromley²; Štefan Matejčík¹; Juraj Országh¹

¹ Comenius University Bratislava, Slovak Republic

² Auburn University, Alabama, USA

The electron-induced fluorescence of carbon monoxide (CO) was studied in a crossed electron and molecule beam experiment using optical emission spectroscopy. CO is one of the dominant carbon bearing molecules in the Universe, especially on extra-terrestrial bodies such as comets or centaurs. Many of the previous publications are focused solely on the Comet Tail system of CO⁺ [1], because of its dominance in higher energy spectra, and the diagnostic of these cometary volatiles is a necessity for solar system formation models [2].

The emission spectrum following electron impact on CO was measured at 5-100 eV within the wavelengths range of 300-1000 nm. The emission bands of CO dominate this spectral region at energies below 20 eV, while the signal from CO⁺ becomes dominant above this energy. The 50 eV spectrum shows a prominent emission of the Comet Tail system of CO⁺ (A²Π - X²Σ⁺), along with a few emission bands of the Baldet-Johnson system of CO⁺ (B²Σ - A²Π⁺) and the emission lines of C I and O I. Excitation-emission functions of several emission bands were measured as well, and their threshold energies were estimated. Additionally, a 3D spectral electron energy map was created, consisting of emission spectra measured at energies ranging from 5 to 100 eV with small energy steps. These data provide detailed information about the excitation-emission functions of all individual transitions in the spectra and their threshold energies. The data is suitable as reference data not only for astrophysical research but for any field utilizing emission spectroscopy.

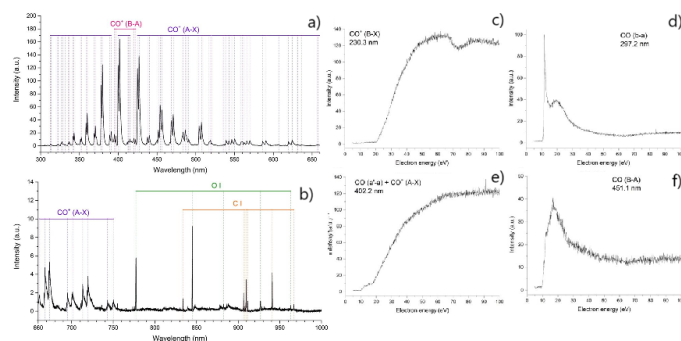


Fig.: The emission spectrum of CO measured by CCD camera at 50 eV (a) within 300-660 nm and (b) within 660-1000 nm. Excitation-emission functions: c) CO⁺ (B²Σ - X²Σ) at 230.3 nm, d) CO (b³Σ⁺ -

$a^3\Pi$) at 297.2 nm, e) CO ($a^3\Sigma^+ - a^3\Pi$) combined with CO⁺ ($A^2\Pi - X^2\Sigma^+$) at 402.2 nm, f) CO ($B^1\Sigma^+ - A^1\Pi$) at 451.1 nm.

This work was supported by the Slovak Research and Development Agency under the Contracts no. SK-PL-23-0050, APVV-19-0386 and APVV-23-0522, Slovak grant agency VEGA under project nr. 1/0553/22. Funded by the EU NextGenerationEU through the Recovery and Resilience Plan for Slovakia under the project No. 09I01-03-V04-00047.

References

- [1] Holland R F and Maier II W B 1972 The Journal of Chemical Physics. 56 11.
- [2] Roth L et al. 2021 Nature Astronomy. 5 1043–1051.

#C50: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Transfer ionization dynamics in collisions involving light ions and helium atoms

Karoly Tokesi¹; N. Bachi²; S. Otranto²

¹ HUN-REN Institute for Nuclear Research

² Instituto de Física del Sur (IFISUR), Departamento de Física, Universidad Nacional del Sur (UNS), CONICET, Av. Alem 1253, Bahía Blanca B8000CPB, Argentina

Transfer ionization (TI) is one of the processes that in the past 20 years allowed elucidating the role of target electron correlation in ion-atom collisions. A decade ago, fully differential cross sections which depend on the emitted electron momentum distribution were measured for H⁺+He collisions at impact energies of 300 and 630 keV. This study allowed determining the dominant role of the initial state correlation over the dynamical correlation experienced by the electron in the reaction region or in the final state [1].

In this work, we explore the dynamics of TI in collisions of H⁺, He²⁺ and Li³⁺ ions with He atoms in the ground state. The impact energy range considered is 10 keV/u–1 MeV/u. Three different variants of the 4-body classical trajectory Monte Carlo (CTMC) method are employed: i) the nCTMC, in which the electrons are considered as independent particles initialized with sequential binding energies of 0.903 a.u. and 2.0 a.u. [2], ii) the Heisenberg core (HC-CTMC), which includes the e-e correlation via the introduction of momentum-dependent stabilizing potentials [3] and iii) the energy-bounded (EB-CTMC) [4], which also includes the full e-e correlation.

We found that according to our correlated model, TI events take mainly place while the projectile is still approaching the target. Moreover, electron capture seems to proceed first with a time difference between peak positions of about 0.5 a.u. of time. Results obtained with the three classical models are analyzed as a function of the impact energy.

The work was supported by the Bilateral relationships between Argentina and Hungary in science and technology (S&T) under project number 2019-2.1.11-TÉT-2020-00202. Work at IFISUR was supported by Grant No. PGI 24/F084, Secretaría General de Ciencia y Tecnología, Universidad Nacional del Sur.

References

- [1] Schöffler M. S. et al 2013 Phys. Rev. A 88 042710
- [2] Olson R. E. 1987 J. Phys. B: At. Mol. Opt. Phys. 20 L809
- [3] Zajfman D. and Maor D. 1986 Phys. Rev. Lett. 56 320
- [4] Cohen J. S. 1996 Phys. Rev. A 54 573

#C51: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Mutual neutralization reactions in collisions between pyrimidine cations and oxygen and chlorine atomic anions

Paola Bolognesi¹; Henning Zettergren²; Lorenzo Avaldi³; Mikael Björkhage²; Mikael Blom²; Laura Carlini¹; Antonella Cartoni⁴; Henrik Cederquist²; Jacopo Chiarinelli¹; Michael Gatchell²; Suvasthika Indrajith²; MingChao Ji²; Paul Martini²; Mathias Poline²; Peter Reinherd²; Stefan Rosén²; Henning Schmidt²; Ansgar Simonsson²; Richard Thomas²

¹ CNR-ISM, Area della Ricerca Roma 1, Monterotondo Scalo (Roma), Italy

² Stockholm University, Stockholm, Sweden

³ CNR-Istituto di Struttura della Materia

⁴ Sapienza Università di Roma, Roma, Italy

The formation and breakage of molecular bonds is at the core of understanding and controlling chemical reactions that determine our life, quality of terrestrial environment as well as evolution of the universe. Depending on the nature of the colliding species different chemical reactions can occur.

In particular, when two molecular ions interact, this can lead to the charge transfer from an anion to a cation, resulting in their mutual neutralisation (MN). Depending on the collision energy this process may lead to the formation of molecular bonds and new species, or to the separation of the two neutral species that are electronically excited. When one of the species is a polyatomic molecule, it can also be ro-vibrationally excited and undergo molecular dissociation as result of internal conversion from an electronic excited state or from head-on collisions (nuclear stopping).

In this work we took advantage of the unique opportunity offered by the cryogenic double electrostatic ion beam storage ring facility DESIREE [1–6] to study mutual neutralization reactions in ~100 meV collisions between pyrimidine cations and atomic anions. In these experiments we performed both two- and three-particle coincidence measurements to explore the charge transfer process at relatively large (oxygen anion) and short (chlorine anion) distances, as well as the following pyrimidine molecule fragmentation. These experiments, supported by Landau-Zener model calculations as well as molecular dynamics simulation, will provide fundamental understanding of biomolecular interactions in relatively complex systems.

References

- [1] R. D. Thomas et al, Review Scientific Instruments 82, 0655112 (2011).
- [2] H. T. Schmidt et al, Review Scientific Instruments 84, 055115 (2013).
- [3] See e.g. J. Grumer et al, Physical Review Letters 128, 033401 (2022) and references therein.
- [4] M. Poline et al, Physical Review Letters 132, 023001 (2024).
- [5] A. Bogot et al, Science 383, 285–289 (2024).
- [6] M. Gatchell et al, Astronomy & Astrophysics 694, A43 (2025).

Acknowledgments

This work is supported by Italian Ministry of Foreign Affairs and International Cooperation”, grant number PGR02090; PNRR-IR project EuPRAXIA Advanced Photon Sources—EuAPS (CUP I93C21000160006, IR0000030); COST Action CA20129 “Multiscale Irradiation and Chemistry Driven Processes and Related Technologies” (MultiChem).

#C52: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Scattering studies between metastable neon and aligned ND3

Viet Le Duc; Andreas Osterwalder

EPFL

The stereodynamics of the $\text{Ne}(3\text{P}_2) + \text{ND}_3 \rightarrow \text{ND}_3^+ / (\text{ND}_2^+ + \text{D}) + \text{e}^-$ reaction is studied in a crossed-beam experiment with aligned ammonia molecules. A sample of aligned ND3 is prepared from a supersonic expansion which is guided and polarized in a curved electrostatic guide, and aligned using a linear electric field in a selected direction. The rotational temperature and degree of alignment are quantified using [2+1] REMPI with linearly polarized light. Metastable neon $\text{Ne}(3\text{P}_2)$ is generated using an Even-Lavie valve coupled to a dielectric barrier discharge and magnetically guided to the reaction zone. Scattering events between $\text{Ne}(3\text{P}_2)$ and ND3 take place in the presence of an electric field to maintain the alignment of ammonia. A short voltage pulse is applied to extract the ionic products which are detected in a time-of-flight mass spectrometer. Preliminary results will be shown to assess the effect of alignment on the branching ratio between the formation of ND3+ and ND2+.

#C53: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Mutual Neutralization with initial-state control

Rachel Poulouse¹; Paul Martini²; Truly Rylander¹; Sadiq Muhamed¹; Mathias Poline¹; Stefan Rosén²; Ansgar Simonsson¹; Michael Gatchell²; Richard Thomas¹; Henrik Cederquist²; Dag Hanstorp³; Henning Zettergren¹; Henning T Schmidt¹

¹ Stockholm University

² Stockholm University, Stockholm, Sweden

³ University of Gothenburg

The DESIREE double cryogenic storage ring at Stockholm University uniquely combines the ability to store and manipulate ions for extended periods of time with the merged-beams configuration allowing studies of sub-eV collisions between ions of opposite charges. By storage alone, molecules are allowed to relax vibrationally and rotationally towards their thermal equilibrium with the cryogenic surroundings, while in particular for small molecular and for atomic ions, the long storage time can be exploited to perform laser-manipulation. In this contribution we present four examples of experiments making use of this unique capability of DESIREE's.

Collision with oppositely charged fullerenes $\text{C}_{60}^+ + \text{C}_{60}^-$ [1], dissociate mutual neutralization in $\text{NO}^+ + \text{O}^-$ collisions [2], MN for metastable and ground state Si^- with Na^+ and K^+ [3] and MN for Au^- ions with Ba^+ with the initial state selected by optical pumping [4].

References

- [1] M Gatchell *et al.* *Astronomy & Astrophysics* **693**, A43 (2025).
- [2] M Poline *et al.* *Phys Rev Letters* **132**, 023001 (2024).
- [3] R Poulouse *et al.* To be submitted.
- [4] R Poulouse *et al.* To be submitted.

#C54: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

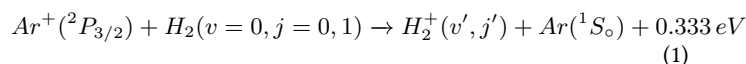
High rotational quantum states in spin orbit state selected charge transfer reaction

Dasarath Swaraj¹; Jerin Judy¹; Fabio Zappa¹; Tim Michaelson¹; Arnab Khan²; Roland Wester¹

¹ University of Innsbruck

² Indian Institute Science Education and Research, Bhopal

Detailed insight into the dynamics of elementary reactions in the gas phase can be obtained from crossed-beam reactive scattering experiments. Angle and energy differential cross-section can be obtained by combining the velocity map imaging (VMI) with crossed-beam scattering[1]. In this contribution, we present the differential cross-section measurement of an ion-molecule charge transfer reaction of argon ions with neutral hydrogen molecules, imaged using VMI with rotationally resolved product distribution significantly improved over our previous study.



The ions were created in the spin-orbit ground state of Ar^+ by Resonance Enhanced Multiphoton ionization (REMPI)[3]. The ions were produced with high energy resolution with our new experimental configuration of electrostatic lenses[4]. Chemical reactions are initiated by the beam of ions intersecting with the beam of neutral molecules generated in a supersonic expansion. The reaction products are collected by the new VMI spectrometer and then detected and imaged. The results show that high product rotational excitation is found, in contrast to reactions of spin-orbit excited $\text{Ar}^+ (^2P_{1/2})$. Quantum scattering calculations are currently underway to describe the reaction.

References

- [1] R. Wester *Phys. Chem. Chem. Phys.*, vol. 16, pp. 396–405, 2014.
- [2] T. Michaelson, B. Bastian, E. Carrascosa, J. Meyer, D. H. Parker, and R. Wester *J. Chem. Phys.*, vol. 147, no. 1, 2017.
- [3] G. Zhang, D. Lu, Y. Ding, L. Guan, S. Han, H. Guo, and H. Gao *Nat. Chem.*, vol. 15, no. 9, pp. 1255–1261, 2023.
- [4] D. Swaraj, T. Michaelson, A. Khan, F. Zappa, R. Wild, and R. Wester *Mol. Phys.*, vol. 122, no. 1-2, p. e2194455, 2024.

#C55: Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Electron-driven reactivity of molecular cations: from mechanisms to cross sections

János Zsolt Mezei¹; Riyad Hassaine²; Rawand Mezlini²; Nicolina Pop³; Kalyan Chakrabarti⁴; Ioan F. Schneider²

¹ HUN-REN Institute for Nuclear Research (ATOMKI), 4026 Debrecen, Bem square 18c, Hungary

² Lab. Ondes et Milieux Complexes, CNRS, Université du Havre, France

³ Dept. of Phys. Foundation of Engineering, Politechnica University Timisoara, Romania

⁴ Dept. of Mathematics, Scottish Church College, Calcutta, India

Electron impact recombination, (ro-)vibrational-, electronic- and dissociative excitation of molecular cations: $\text{AB}^+ + \text{e}^- \rightarrow \text{AB}^*$, $\text{AB}^{**} \rightarrow \text{A} + \text{B}$ (DR) or $\text{AB}^{+*} + \text{e}^-$ (RV(d)E) or $\text{A} + \text{B}^+ + \text{e}^-$ (DE) are in the heart of the molecular reactivity in all cold ionized media [1], being major charged particles destruction reactions and producing often atomic species in

metastable states, inaccessible through optical excitations. They involve super-excited molecular states undergoing predissociation and autoionization, having thus strong resonant character. The Multichannel Quantum Defect Theory (MQDT) [1,2] based methods are the most suitable approaches for these processes, capable to account the strong mixing between ionization and dissociative channels, open - direct mechanism - and closed - indirect mechanism, via capture into prominent Rydberg resonances correlating to the ground and excited ionic states, and the rotational effects. These features will be illustrated for several cations of high astrophysical, planetary atmosphere and fusion edge plasma relevance such as SH^+ [3], NS^+ [4] and BeH^+ [5], comparisons with other existing theoretical and experimental results also being performed. Advancement in the theoretical treatment - different dissociation channels or the isotopic effects for diatomic and polyatomic systems like NeH^+ [6], H_2^+/HD^+ and N_2H^+ [7], or C_2H^+ etc. - will be presented.

- [1] I. F. Schneider, O. Dulieu, J. Robert, eds., EPJ Web of Conferences 84 (2015).
- [2] J. Zs. Mezei et al, ACS Earth and Space Chem 3, 2276 (2019).
- [3] J. Boffelli et al, MNRAS 522, 2259 (2023).
- [4] R. Hassaine et al, J. Phys. B: At. Mol. Opt. Phys. 57, 165201 (2024).
- [5] E. Djuissi et al, PCCP 26, 18311 (2024).
- [6] R. Hassaine et al, J. Chem. Phys. 162, 134302 (2025).
- [7] J. Zs. Mezei et al, EPJST 232, 1967 (2023).

#C56: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Xenon photoionization in the vicinity of 4d giant resonance and Cooper minimum using an XUV-NIR pump-probe experiment at FLASH

Igor Litvinyuk

Griffith University

The relaxation processes in atomic xenon following core ionization of the 4d and 4p subshells by extreme ultraviolet (XUV) pulses from a free-electron laser (FLASH: FL26 beamline) are investigated using ion time-of-flight spectroscopy (see [1] for detailed description of the experimental setup). We compare the dynamics following ionization and Auger-Meitner decays at 90-eV photon energy, i.e., near the giant resonance, with those at 160 eV, near the Cooper minimum, where cross sections for photoionization of the 4d and 4p subshells are similar. Final states with charges higher than 4 show signatures of sequential absorption of two XUV photons, followed by subsequent Auger-Meitner decay. The averaged lifetimes of some important excited states are measured in a two-color XUV-pump-near-infrared-probe experiment (XUV pulse duration is (20±10) fs and 800 nm NIR pulse duration is (15±3) fs). A transient enhancement in the ion yield of Xe^{5+} with an average lifetime of (49 ± 3) fs is obtained, attributed to transient intermediate states following the decay of 4d double-core-hole states [2]. This lifetime for Xe^{5+} is twice as short as observed earlier. A different decay channel of Xe^{6+} was observed, most likely arising from NIR-induced double ionization of doubly excited states of Xe^{4+} . This work demonstrates that utilizing intense XUV and x-ray sources, such as FEL, enables the selective population of core-hole states and with NIR pulses allows studying decay dynamics in atoms and molecules.

References

- [1] Atia-Tul-Noor et al. 2024 Opt. Express 32 6597
- [2] Kumar S et al. 2024 Phys Rev A 110 063104

#C57: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Ionization Induced Dynamics

Daniel Strasser

Institute of chemistry, The Hebrew University of Jerusalem, Isarel

In recent years, my group explores intramolecular and intermolecular charge-transfer mechanisms in various ionization and neutralization processes.[1,2] Here, I will present ultrafast EUV pump –EUV probe studies of the $(\text{CO}_2)_2^+$ dynamics that we initiated by photoionization of neutral carbon dioxide dimers and probed by Coulomb explosion imaging as a function of the pump-probe time delay.[3] By comparing the experimental data with AIMD simulations we revealed unexpected asymmetric structural rearrangement from the slipped-parallel (C2h) geometry of the neutral CO_2 dimer towards a T-shaped (C2v) structure on the ~100 fs timescale. These results are surprising because of the most stable slipped-parallel (C2h) structure of the ionic dimer. I will also show that excited states of the ionized CO_2 dimer can exhibit formation of a CO_3 moiety in the C_2O_4^+ complex that can persist even after a suitably time-delayed second photoionization in a metastable $\text{C}_2\text{O}_4^{2+}$ dication. Our results suggest that charge asymmetry plays an important role in the ionization-induced dynamics in such dimers that are present in CO_2 rich environments, as well as in other symmetric dimer and cluster systems.

References

- [1] K. Gope, et al., An “inverse”harpoon mechanism, Science Advances,8, 39 (2022)
- [2] A. Bogot, et al., The mutual neutralization of hydronium and hydroxide, Science, 383,285 (2024)
- [3] E. Livshits, et al., Symmetry-breaking dynamics of a photoionized carbon dioxide dimer, Nature Communications, 6322 (2024)

#C58: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Real time observation of the formation of Li^+ -benzene complexes

Christian Engelbrecht Petersen¹; Jeppe Kjædegaard²;
Simon Høgh Albrechtsen³; Florent Calvo⁴; Henrik
Stapelfeldt²

¹ Aarhus University, Department of Physics and Astronomy

² Aarhus University, Department of Chemistry

³ Aarhus University, Department of Chemistry

⁴ Université Grenoble Alpes

It is challenging to measure the real time bond formation between two atoms or molecules because of the difficulty in preparing such a system in a well-defined starting geometry. A second challenge is to measure when the reactants meet since this is determined by diffusion, a process which is not easily controlled. Previous work have overcome these difficulties by preparing the system as a weakly bonded van der Waals complex, and then initialising the reaction by photoionisation [1].

In this work, we show real-time measurements of diffusion limited formation of Li^+ -benzene complexes. The initial system is prepared using a helium nanodroplet housing a benzene molecule at its centre and and lithium atom on its surface. The atom-molecule separation is determined by the radius of the droplet which, in our experiments, can be controlled to be in the range 35-55 Å. We initialise the diffusion process at a well-defined time by ionising the lithium atom through a multi-photon ionisation process using a 800 nm, 50 fs laser pump pulse. Following the ionisation, the newly formed lithium ion is pulled

into the droplet, and a subsequent ionisation of the benzene molecule would lead to measurement of the solvation rate of the ion as found in [2,3].

However, not ionising the benzene molecule will allow the lithium ion to meet benzene at the centre of the droplet and form a complex. We terminate the diffusion of the lithium ion –whether it has reached the benzene molecule or not –at a well-defined time by ionising benzene with a 400 nm, 70 fs laser probe pulse. This triggers a strong Coulomb repulsion between the two positively charged ions, and they will be ejected from the droplet.

Using a VMI spectrometer, we detect a 180 degree coincidence angle between benzene and lithium ions only after the complex has formed. This allows us to determine at which time the complex has formed by varying the delay of the probe pulse with respect to the pump pulse. In extension, this allows us to determine the diffusion rate, i.e. the speed at which the lithium ion moves through the droplet, by varying the size of the helium droplets. We found the diffusion rate of Li^+ through the droplets to be 22 ± 3 m/s.

- [1] Kyung Hwan Kim *et. al.*, Nature 518, 385–389 (2015)
 [2] Simon H. Albrechtsen *et. al.*, Nature 623, 319–323 (2023)
 [3] Simon H. Albrechtsen *et. al.*, arXiv:2502.11783

#C59: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Driving and Imaging Achiral-to-Chiral Transitions in an All-Optical Setup

Edward Binns¹; Justas Terentjevas²; Laura Rego³; Andrés Ordóñez⁴; David Ayuso⁵

¹ Imperial College London

² Max-Born-Institut

³ Instituto Madrileño de Estudios Avanzados en Nanociencia (IMDEA Nano)

⁴ Imperial College London / Freie Universität Berlin

⁵ Imperial College London, Department of Chemistry, UK

Synopsis: We show how to imprint the handedness of locally chiral light into achiral matter, and how to monitor such achiral-to-chiral phase transitions in an all-optical setup. Our proof-of-principle simulations reveal that the hydrogen atom undergoes ultrafast and highly nonlinear chiral electron dynamics when exposed to an intense, ultrashort, locally chiral laser pulse, giving rise to chiral high harmonic generation. Whatmore, the atom remains in a chiral superposition of stationary states after the pulse is gone, emitting chiral free-induction decay radiation which reveals the imprinted handedness.

Synthetic chiral light, introduced in [2], enables ultrafast and highly efficient imaging of molecular chirality. It is locally chiral: the tip of the electric-field vector draws a chiral (3D) Lissajous figure in time, at each point in space. Since its chirality is preserved within the electric dipole approximation, it achieves maximum chiral sensitivity. Interestingly, such tailored light can also be used to create chiral electronic states in atoms [3], which emit chiral photoelectron currents and exhibit photoelectron circular dichroism [3].

We demonstrate how synthetic chiral light, both locally and globally chiral [2], imprints and records chirality in achiral media. By driving ultrafast chiral electron motion in initially achiral systems, such as atoms, we induce ultrafast achiral-to-chiral phase transitions.

We solved the time-dependent Schrödinger equation for a hydrogen atom exposed to an ultrashort, intense, locally chiral field. The laser drives ultrafast chiral electron motion at its fundamental frequencies (800 nm and 400 nm) leading to the generation of high-frequency components creating a chiral structure in time. These components give rise to chiral high harmonic generation (HHG). After the pulse the atom remains in a chiral coherent superposition of stationary states, and thus the electron continues to undergo ultrafast time dependent chiral dynamics. Changing the relative phases of the components of

the field varies the phase of our imprinted dynamics. We will introduce a novel chiral measure to describe the instantaneous chirality of the dipole motion. This measure accompanies the chiral correlation functions defined for our locally chiral field and describe the strength of the interaction between the field and chiral matter. This allows for robust characterization of our elliptically rotating time-dependent chirality.

We believe that this work creates exciting opportunities for driving and monitoring achiral-to-chiral phase transitions in all-optical setups, also in complex systems, as well as for driving chiral photo-chemical reactions using achiral reagents.

References

- [1] Ordonez A F and Smirnova O 2019 Phys. Rev. A 99 043416
 [2] Ayuso D *et al* 2019 Nat. Photon. 13 866
 [3] Mayer N *et al* 2022 Phys. Rev. Lett. 129 243201

• E-mail: edward.binns19@imperial.ac.uk

#C60: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

RABBITT including Higher-Order Processes

Luke Roantree; Hugo van der Hart; Andrew Brown

Queen's University Belfast

The RABBITT (Reconstruction of Attosecond Beating by Interference of Two-photon Transitions) technique is a foundational tool in attosecond science, enabling the precise extraction of amplitude and phase information from photoelectron spectra. Traditional RABBITT is limited to weak infrared (IR) fields and two-photon pathways. We have generalised the framework through the RABBITT with Higher Order Processes (RABBITT-HOP) formalism. In this work we show how RABBITT-HOP can explain results from experiments and simulations with helium, and how, even at moderate IR intensities, the signatures of higher-order processes can be extracted from photoelectron spectra.

An attosecond pulse train is constructed to target the $1s4p$ and $1s5p$ states in He, such that the resonant pathways imprint the characteristic ‘antiresonance’ into the phase extracted from the neighbouring sideband [1]. RABBITT-HOP then predicts that the same resonant pathways will contribute to higher-lying sidebands/mainbands via four-photon transitions, and that the antiresonance should manifest in the phase of higher frequency oscillations via four photon transitions.

We verify these predictions with R-matrix with time-dependence [2] simulations of He, and identify the resonant signature in photoelectron signals in multiple sidebands and mainbands. Via analysis of photo-electron angular distributions (PAD) we provide further evidence of these higher-order processes [3]. Delay-resolved anisotropy parameters to reveal the role played by the g_0 partial waves (reached by four-photon transitions) to the spectral phase shift in the PAD. Even though the amplitude of the g_0 wave is tiny compared to the s and d_0 waves, its *interference* is detectable. This provides an efficient method to visualise partial wave contributions beyond the perturbative regime.

- [1] L Drescher *et al.*, Phys. Rev. A **105**, L011101 (2022).
 [2] A C Brown *et al.*, Comp. Phys. Commun. **250**, 107062 (2020).
 [3] W Jiang *et al.*, Nat. Comm. **16**, 381 (2025).

#C61: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

First-principles evaluation of the complete HHG observable in solids

Dieter Bauer; Francisco Navarrete

Institute of Physics-University of Rostock

High harmonic generation (HHG) occurs when an intense infrared laser interacts with matter, producing radiation at integer multiples of the laser's fundamental frequency [1]. It was first studied in atomic and molecular gases [1] and later extended to solids [2], enabling compact ultrafast light sources. Recent interest in the quantum properties of the driving pulse [3,4], together with persistent discrepancies between theoretical and experimental HHG spectra in solids [5,6], has driven the development of new computational approaches [4]. We compare the conventional HHG observables [7] with an alternative formulation that treats the light field quantum mechanically and includes terms typically neglected in the standard approach. We find that both methods reproduce the main spectral features - a plateau and odd harmonics - but differ in other qualitative aspects. The fully quantum mechanical observable yields sharper spectral components in solids, although its broad features in the interband region remain similar to the conventional result. In the intraband region, however, the two approaches produce qualitatively different spectra. We attribute this difference to contributions from initially unoccupied electronic bands that are omitted in the conventional observable.

[1] M. Lewenstein *et al.*, *Phys. Rev. A* **49**, 2117 (1994)

[2] S. Ghimire *et al.*, *Nat. Phys.* **7**, 138 (2011)

[3] M. Lewenstein *et al.*, *Nat. Phys.* **17**, 1104 (2021)

[4] Goriach, A., Neufeld, O., Rivera, N. *et al.* *Nat Commun* **11**, 4598 (2020).

[5] I. Floss *et al.*, *Phys. Rev. A* **97**, 011401(R) (2018)

[6] Cavaletto *et al.* *Nat. Rev. Phys.* **7**, 38 (2025)

[7] B. Sundaram and P. W. Milonni, *Phys. Rev. A* **41**, 6571(R) (1990)

#C62: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Partial-wave transitions in attosecond time delays and separability of Wigner delays

Franck Lépine¹; Jakub Benda²; Saikat Nandi¹; Sreelakshmi Palakkal¹; Vincent Lorient¹; Zdeněk Mašín²

¹ Université Claude Bernard Lyon 1, CNRS, Institut Lumière Matière, UMR5306, F-69100 Villeurbanne, France

² Institute of Theoretical Physics, Faculty of Mathematics and Physics, Charles University, V Holešovičkách 2, Prague 8, 180 00, Czechia

In our recent work [1] we develop a method for accurate calculation and interpretation of photoionization delays in atoms and molecules measured using multiphoton interference techniques, with a particular focus on the Reconstruction of Attosecond Beating by Interference of Two-photon Transitions (RABITT).

Specifically, we investigate implications of a “two-harmonic RABITT” experiment performed in argon, featuring a single central sideband, two mainbands and two outer sidebands, each alone well usable for extraction of compatible timing information.

Current methods, which rely on separation of the measurable delays into Wigner-like delay and continuum-continuum delay τ_{CC} , often fall short at low photoelectron kinetic energies and fail to capture the correct angular dependencies. To address this, we have developed an

innovative analytical approach that not only predicts correction terms accurately even at very low energies but also incorporates the angular dependence of the continuum-continuum delay. Our method is computationally efficient and has been rigorously validated against state-of-the-art *ab initio* calculations using the stationary multiphoton R-matrix method [2] and the R-matrix with time-dependence (RMT) [3].

By introducing a partial-wave-resolved continuum-continuum contribution, we achieve a precise modeling of the infrared field's influence on different photoelectron partial waves. This advancement allows for a clearer interpretation of both angularly resolved and angle-integrated RABITT delays, demonstrating excellent agreement with the full above-threshold perturbation theory. Our experimental setup, utilizing a simplified RABITT configuration, effectively isolates higher-order multiphoton pathways, offering a promising method for analyzing complex molecular photoionization spectra.

[1] J Benda *et al.*, *Phys. Rev. A* **111**, 013110 (2025).

[2] J Benda, Z Mašín, *Sci. Rep.* **11**, 11686 (2021).

[3] A C Brown *et al.*, *Comput. Phys. Commun.* **250**, 107062 (2020).

#C63: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Ultrafast correlation dynamics during high-harmonic generation in multi-electron atoms

Katharina Buczolic¹; Takeshi Sato²; Kenichi L. Ishikawa²; Fabian Lackner¹; Joachim Burgdörfer¹; Iva Březinová¹

¹ Institute for Theoretical Physics, Vienna University of Technology, 1040 Vienna, Austria, EU

² Graduate School of Engineering and Photon Science Center, School of Engineering, The University of Tokyo and Research Institute for Photon Science and Laser Technology, The University of Tokyo

We study the role of electronic correlations during high harmonic generation (HHG) in multi-electron atoms. Originally viewed as a process involving one single active electron, the influence of multi-electron effects on the HHG spectrum has lately been extensively studied (see e.g. [1, 2]). We quantify the time-dependence of electron-electron correlations on ultrafast time scales using correlation measures from quantum information theory.

By explicitly solving the time-dependent Schrödinger equation with the multi-configurational time-dependent Hartree-Fock (MCTDHF) method [3], we obtain fully correlated results for He, Ne, Be and Mg. Using driving fields adjusted to the ionization potential of each atom, such that the driving occurs in the strong-field regime and double-ionization is negligible, we compare the HHG yields for the different atomic species.

We find prominent features of the influence of correlations on both the tunneling as well as the recombination step. While during tunneling the correlations systematically increase for noble gas atoms (He, Ne), they decrease for alkaline earth atoms (Be, Mg). During recombination we find that the correlated electrons oscillate out of phase relative to each other. Both processes imprint distinct signatures of correlations on the HHG spectrum.

[1] A. D. Shiner *et al.*, *Nature Phys* **7**, 464–467 (2011).

[2] Y. Li *et al.*, *Phys. Rev. A* **99**, 043401 (2019).

[3] T. Sato *et al.*, *Phys. Rev. A* **94**, 023405 (2016).

#C64: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong fields

Femtosecond timed imaging of rotation and vibration of alkali dimers on the surface of helium nanodroplets

Henrik Høj Kristensen¹; Lorenz Kranabetter¹; Areg Ghazaryan²; Nicolaj Jyde¹; Jeppe Christensen¹; Emil Hansen³; Constant Schouder⁴; Frank Jensen¹; Robert Zillich⁵; Mikhail Lemeshko²; Henrik Stapelfeldt¹

¹ Department of Chemistry, Aarhus University

² Institute of Science and Technology Austria

³ Department of Physics, Aarhus University

⁴ ISMO, CNRS, Université Paris-Saclay

⁵ Institute for Theoretical Physics, Johannes Kepler Universität

Alkali dimers, Ak_2 , residing on the surface of helium nanodroplets, are set into rotation and vibration, through the dynamic Stark effect, by a moderately intense 50-fs pump pulse. Coulomb explosion of dimers in the singlet $X^1\Sigma_g^+$ and triplet $a^3\Sigma_u^+$ state [1, 2], induced by an intense, delayed femtosecond probe pulse, is used to record the time-dependent nuclear motion.

Concerning rotation, the measured alignment traces for Na_2 , K_2 , and Rb_2 show distinct periodic features that differs qualitatively from the well-known alignment dynamics of linear molecules in either the gas phase or dissolved in liquid helium [3]. Instead, the observed alignment dynamics of Na_2 and K_2 in the $a^3\Sigma_u^+$ state and of K_2 and Rb_2 in the $X^1\Sigma_g^+$ state agree with that obtained from a 2D rigid rotor model, strongly indicating that the rotation of each dimer occurs in a plane - defined by the He droplet surface [4, 5].

Concerning vibration, the Coulomb explosion probe method enables us to measure the distribution of internuclear distances as a function of time. For K_2 in the $a^3\Sigma_u^+$ state, we observe a distinct oscillatory pattern caused by a two-state vibrational wave packet in the initial electronic state of the dimer. The wave packet is imaged for more than 250 vibrational periods with a precision better than 0.1 Å on its central position. Unlike the rotational motion, the vibration of the dimer is essentially unaffected by the presence of the He droplet [6].

References:

- [1] H. H. Kristensen, et al. Phys. Rev. Lett. **128** (2022), 093201
- [2] H. H. Kristensen, et al. Phys. Rev. A **107** (2023), 023104
- [3] A. S. Chatterley, et al. Phys. Rev. Lett. **125** (2020), 013001
- [4] L. Kranabetter, et al. Phys. Rev. Lett. **131** (2023), 053201
- [5] H. H. Kristensen, et al., In preparation. (Available at arXiv:2502.14521 [physics.atom-clus])
- [6] N. K. Jyde, et al. J. Chem. Phys. **161** (2024), 224301

#C65: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Magnetic field system for AQuRA transportable quantum clock

Sławomir Bilicki; Adam Ledziński; Piotr Morzyński; Michał Zawada

KL FAMO, Institute of Physics, Nicolaus Copernicus University in Toruń

We present the magnetic system constructed for the state-of-the-art 5×10^{-18} fractional frequency uncertainty Sr transportable clock developed within the “Advanced Quantum Clock For Real-World Appli-

cations” project. The system includes a compact permanent-magnets Zeeman slower, a pair of Helmholtz coils for atom trapping, and a compact set of compensation coils used to cancel out external magnetic fields. The longitudinal Zeeman slower is designed to minimize the magnetic field at the output of the atomic beam, disturbing the field at the centre of the science chamber at the level of 10^{-7} T. The coils are controlled by programmable drivers modules mounted in Sinara 3HU 19”EuroRack-size crate. The drivers provide up to 100 A and 3×3 A of current for MOT coils and compensation coils, respectively, allows for fast switching between desired levels, a linear ramp of arbitrary time, and switching between Helmholtz and anti-Helmholtz configuration. The AQuRA project has received funding from the European Union’s Horizon Europe research and innovation programme under grant agreement No 101080166 (AQuRA project).

#C66: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Reduced instability in a high-accuracy $^{115}\text{In}^+ / ^{172}\text{Yb}^+$ Coulomb crystal optical clock

Jonas Keller; H. Nimrod Hausser; Ingrid M. Richter; Shobhit Saheb-Dey; Tanja E. Mehlstäubler

Physikalisch-Technische Bundesanstalt

Mixed-species Coulomb crystal operation can reduce both statistical and systematic uncertainties in optical clocks. Increased clock ion numbers provide a lower quantum projection noise limited instability and are the prerequisite for various advanced interrogation schemes, while auxiliary ions can be used for sympathetic cooling and systematic shift characterization.

We operate a clock based on a linear chain of $^{115}\text{In}^+$ (clock) and $^{172}\text{Yb}^+$ (auxiliary) ions, which we have identified as a favorable system for high-accuracy multi-clock-ion operation [1], capable of reaching a fractional systematic uncertainty below 1×10^{-19} [2].

With an evaluated uncertainty of 2.5×10^{-18} , the clock has participated in the first inter-species frequency ratio measurement [3] to fulfill the $< 5 \times 10^{-18}$ requirement stated by the CCTF roadmap toward the redefinition of the second [4].

The instability in multi-clock-ion operation was initially limited by unfavorable scaling of dead time due to a state preparation scheme based on spontaneous decay [5]. We have therefore implemented a repumping step using the $^3\text{P}_0$ to $^1\text{P}_1$ M1 transition at 482 nm, which reduces the effective $^3\text{P}_0$ lifetime to 3.5 ms. The instability now follows the expected $1/\sqrt{N}$ scaling with ion number N and reaches $\sigma_y = 6(2) \times 10^{-16}/\sqrt{t}$ in operation with 4 In^+ ions.

[1] N. Herschbach et al., Appl. Phys. B **107**, 891 (2012)

[2] J. Keller et al., Phys. Rev. A **99**, 013405 (2019)

[3] H. N. Hausser et al., Phys. Rev. Lett. **134**, 023201 (2025)

[4] N. Dimarcq et al., Metrologia **61**, 012001 (2024)

[5] J. Keller et al., J. Phys.: Conf. Ser., **2889**, 01205 (2024)

#C67: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Absolute quantum gravimeter and gradiometer for field applications

Taeg Yong Kwon; Sang-Bum Lee; Sangwon Seo; Sang Eon Park; Sang Lok Lee; Hyun-Gue Hong; Jae Hoon Lee; Young-Ho Park; Seji Kang; Meung Ho Seo

Korea Research Institute of Standards and Science

An absolute atomic gravimeter and gradiometer based on atom interferometry have emerged as powerful tools for measuring the mass distribution beneath the Earth's surface. The spatial and temporal variations in gravity can be measured precisely with quantum gravimeters and gradiometers. These precise gravity measurements provide valuable information for geosciences, including geophysics, hydrology, volcanology, and underground resource exploration.

We report on the development of a quantum gravimeter and gradiometer based on an atom interferometer for field applications. The uncertainty of the gravimeter, based on Rb atoms, is estimated to be below 30 nm/s², primarily limited by wavefront distortion effects. To improve the uncertainty to below 10 nm/s², we are developing a Cs gravimeter of the atomic fountain type. Furthermore, to enable precise gravity measurements, we are developing a gravity gradiometer that consists of two identical gravimeters installed in one system.

In the presentation, we will discuss the uncertainty evaluation of the Rb gravimeter and introduce recent progress in the development of the Cs atomic fountain gravimeter and the Rb gradiometer

#C68: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Optical clock spectroscopy with Sr ensembles in reconfigurable tweezer arrays

Jack Segal¹; Ryuji Moriya¹; Mitchell Walker¹; Liam Gallagher¹; Matthew Hill¹; Frederic Leroux¹; Zhongxiao Xu²; Matthew Jones¹

¹ Durham University

² Shanxi University

We report on progress towards implementing Rydberg-based spin squeezing protocols [1] using small ($N < 10$) ensembles of Sr atoms in magic-wavelength optical tweezers. Highly-excited Rydberg states provide new ways to engineer entanglement in optical frequency standards such as Sr and Yb atomic clocks, with the first results using single atoms in tweezer arrays appearing recently [2, 3]. A similar protocol was implemented using a 1D array of ensembles of Cs atoms [4]: our current goal is to examine whether a similar approach using smaller ensembles could be used in Sr tweezer experiments.

We will describe our experiments with ensembles of 88Sr atoms trapped in long working distance optical tweezers [5] at the 813 nm magic wavelength. Our larger tweezer waist (2 microns) allows the collisional blockade to be circumvented such that we can load small ensembles into each site of a 2D reconfigurable array (site spacing ~6 microns). We demonstrate a novel technique implemented in our experiment to load spatially large (100 microns by 200 microns) 2D tweezer arrays with arbitrary atom number distributions across sites. We will present results on site-resolved spectroscopy of the 1S0-3P0 clock transition as a function of the number of atoms per tweezer site, alongside interpretation in terms of density-dependent collisions. As outlook, we intend to perform precision Rydberg spectroscopy from the 3PJ states in individual tweezers.

- [1] L. I. R. Gil et al., PRL 112 (2014)
- [2] G. Bornet et al., Nature 621 (2023)
- [3] W. J. Eckner et al., Nature 621 (2023)
- [4] J. A. Hines et al., PRL 131 (2023)
- [5] N. C. Jackson et al., SciPost Phys. 8 (2020)

#C69: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Searching for dark matter with a spin-based interferometer

Daniel Gavilan-Martin¹; Grzegorz Łukasiewicz²; Mikhail Padniuk²; Emmanuel Klinger³; Magdalena Smolis²; Nathaniel L. Figueroa¹; Derek F. Jackson Kimball⁴; Alexander O. Sushkov⁵; Szymon Pustelny²; Dmitry Budker¹; Arne Wickenbrock⁶

¹ Johannes Gutenberg University

² Jagiellonian University

³ Institut FEMTO-ST - CNRS

⁴ California State University –East Bay, Hayward

⁵ Boston University

⁶ Johannes Gutenberg

Axion-like particles (ALPs) are well-motivated extensions to the Standard Model and could form a dark matter field that oscillates at a frequency proportional to their mass. Because the value of the ALP mass could be anywhere in the range of 10^{-22} to 10 eV/c², it is important to search across a broad frequency range. We present a new search for ALPs over nine orders of magnitude in mass using a pair of atomic comagnetometers operating as a dark matter field interferometer [1]. Our sensors use alkali metal and noble gas atoms in the same vapor cell, where spin interactions between the atoms suppress the response of the sensor to slow (~ 1 Hz) magnetic fluctuations, while enabling sensitivity to spin-dependent interactions [2]. Data from the two comagnetometers, located in Kraków, Poland, and Mainz, Germany, allow us to search for a correlated ALP-induced pseudomagnetic interaction with atomic spins. We model the coherence properties of the ALP field and construct a signal model that remains valid across nine orders of magnitude in frequency, allowing us to take advantage of the expected spatio-temporal correlations in the data. No significant ALP candidate was found, and we set new limits on ALP couplings to neutrons, protons, and electrons, improving previous constraints by up to three orders of magnitude.

[1] D. Gavilan-Martin, G. Łukasiewicz, M. Padniuk, E. Klinger, M. Smolis, et al., Searching for dark matter with a 1000 km baseline interferometer (2024), arXiv:2408.02668.

[2] T. W. Kornack and M. V. Romalis, Dynamics of two overlapping spin ensembles interacting by spin exchange, Phys. Rev. Lett. 89, 253002 (2002).

#C70: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Self-ordering, cooling, and lasing in an ensemble of clock atoms

Anna Bychek¹; Helmut Ritsch²; Laurin Ostermann

¹ Institute for Theoretical Physics, University of Innsbruck

² Theoretische Physik

Active atomic clocks are predicted to provide far better short-term stability and robustness against thermal fluctuations than typical feedback-based optical atomic clocks. However, continuous laser operation using an ensemble of clock atoms still remains an experimentally challenging task. We study spatial self-organization in a transversely driven ensemble of clock atoms inside an optical resonator and coherent light emission from the cavity. We focus on the spectral properties of the emitted light in the narrow atomic linewidth regime, where the phase coherence providing frequency stability is stored in the atomic dipoles rather than the cavity field. The atoms are off-resonantly driven by a standing-wave coherent laser transversely to the cavity axis allowing for atomic motion along the cavity axis as well as along the pump. In order to treat larger atom numbers we employ a second-order cumulant expansion which allows us to calculate the spectrum of the cavity light field. We identify the self-organization threshold where the atoms align themselves in a checkerboard pattern, thus maximizing light scattering into the cavity, which simultaneously induces cooling. For a larger driving intensity, more atoms are transferred to the excited state, reducing cooling but increasing light emission from the excited atoms. This can be enhanced via a second cavity mode at the atomic frequency spatially shifted by a quarter wavelength. For large enough atom numbers we observe laser-like emission close to the bare atomic transition frequency.

#C71: Quantum technologies, quantum optics, cavity QED, quantum information

Miniature quantum devices build of dipole coupled nano arrays of quantum emitters

Helmut Ritsch¹; Raphael Holzinger²

¹ Theoretische Physik

² University of Innsbruck

An array of closely spaced, dipole coupled quantum emitters exhibits collective energy shifts as well as super- and sub-radiance with characteristic tailorable spatial radiation patterns. As a striking example we identify a sub-wavelength sized ring of exactly 9 identical dipoles with an extra identical emitter with an extra loss channel at the center as the most efficient configuration to deposit incoming photon energy to center without reemission. For very tiny structures below a tenth of a wavelength a full quantum description exhibits an even larger enhancement than predicted from a classical dipole approximation. Adding gain to such systems allows to design minimalistic classical as well as non-classical light sources.

On the one hand this could be the basis of a new generation of highly efficient and selective nano antennas for single photon detectors for microwaves, infrared and optical frequencies, while on the other hand it could be an important piece towards understanding the surprising efficiency of natural light harvesting molecules.

Ref: Holzinger, Raphael, Mariona Moreno-Cardoner, and Helmut Ritsch. "Nanoscale continuous quantum light sources based on driven dipole emitter arrays", Appl. Phys. Lett. 2021

#C72: Quantum technologies, quantum optics, cavity QED, quantum information

Efficient computation of the classical bound of Bell correlation and prepare-and-measure witnesses in parallel environments

István Márton

HUN-REN Institute for Nuclear Research

We present a program speeding up the brute force calculation of the L_d norms of an $n \times m$ matrix M . The L_1 norm stands for the local bound of the Bell expression [1], meanwhile, L_d norms where $d \geq 2$ are the classical d -dimensional bounds of the prepare-and-measure (PM) witness [2]. In both cases, we assume binary outputs. These norms are of interest in the field of communication complexity, the Grothendieck constant, or in graph theory. The effectiveness of our implementation is based on two factors. On the one hand, our code capitalizes on the efficient implementation of the algorithm calculating the L_d norms using special mathematical and programming techniques. On the other hand, our code is implemented in the C programming language with OpenMP, MPI, or CUDA exploiting the advantages of shared or distributed parallelism, or capable of utilizing massively parallel platforms, namely Graphics Processing Units (GPUs).

[1] P. Diviánszky, E. Bene and T. Vértesi, Phys. Rev. A, 96 (2017) 012113

[2] P. Diviánszky, I. Márton, E. Bene and T. Vértesi, Scientific Reports, 13 (2023) 13200

#C73: Quantum technologies, quantum optics, cavity QED, quantum information

Non-Destructive Photon Number Measurement Using Quantum Phase Estimation

Lucas Santos¹; Ciro Diniz¹; Gabriel Fernandes¹; Luiz Solak¹; Daniel Rossatto²; Celso Villas-Boas¹

¹ Departamento de Física - UFSCar

² Universidade Estadual Paulista (UNESP), Instituto de Ciências e Engenharia, Itapeva

This work explores the application of the Quantum Phase Estimation (QPE) algorithm for the non-destructive measurement of the average photon number $\langle n \rangle$ in a free field, using qubits to capture the decay dynamics of the quantum field. The protocol is implemented with 5 qubits, achieving high precision in estimating the phase associated with $\langle n \rangle$, with uncertainties of $1/2^{32}$. An effective Hamiltonian model of system evolution and dynamics is simulated using the Monte Carlo method, reproducing decay via quantum jumps. The obtained results are compared with semiclassical solutions, highlighting QPE capability to distinguish quantum characteristics of the field. This study demonstrates the feasibility of QPE for non-destructive quantum measurements, motivating the implementation of the protocol in available experimental platforms.

#C74: Quantum technologies, quantum optics, cavity QED, quantum information

Efficient excitation energy transfer in a bio-inspired stacked nanoscale quantum emitter ring geometry

Arpita Pal¹; Raphael Holzinger¹; Maria Moreno-Cardoner²; Helmut Ritsch¹

¹ Institut für Theoretische Physik, Universität Innsbruck

² Universitat de Barcelona

Nature relies on biological light-harvesting (LH) complexes to capture and transfer solar energy to the reaction center with supreme efficiency. These LH complexes can be modeled theoretically as sub-wavelength rings of optical dipoles [1-4] which partially explains their outstanding collective optical properties. Taking inspiration from the oligomeric geometry of biological LH2 complexes [5, 6], here theoretically we propose a nonameric stacked three-dimensional (3D) ring geometry formed of two-level atoms with a diameter of 400 nm [7]. This 3D ring structure enables efficient inter-ring excitation transfer, in particular from the sparse to dense ring layer, when operated at zero temperature [7]. Our findings will be useful for designing artificial nanophotonic geometries utilizing different platforms operating at cryogenic temperature, where the interacting dipole description is both valid and dominant, to facilitate efficient energy transfer.

- [1] M. Moreno-Cardoner *et al.*, Phys. Rev. A **100**, 023806 (2019)
- [2] J. A. Needham *et al.*, New J. Phys. **21**, 073061 (2019)
- [3] V. Scheil *et al.*, Nanomaterials **13**, 851 (2023)
- [4] R. Holzinger *et al.*, Optica Quantum **2**, 57 (2024)
- [5] G. McDermott *et al.*, Nature **374**, 517 (1995)
- [6] D. Montemayor *et al.*, J. Phys. Chem. B **122**, 3815 (2018)
- [7] A. Pal *et al.*, arXiv:2409.15288 (2024)

Grant acknowledgments:

This research was funded in whole or in part by the Austrian Science Fund (FWF) 10.55776/ESP682. We also acknowledge support from Forschungsgruppe FG 5 (FWF); 10.55776/W1259 (FWF) (R.H.); 10.55776/COE1 (quantA) (R.H.); Grant No. PID2020-114626GB-I00 from the MICIN/AEI/10.13039/501100011033 (Government of Spain) (M.M.-C.).

#C75: Quantum technologies, quantum optics, cavity QED, quantum information

Demonstration of strong coupling of a subradiant atom array to a cavity vacuum

András Dombi; András Vukics; Árpád Kurkó; Bálint Sárközi; Bence Gábor; Dániel Varga; David Nagy; F. I. B. Williams; K. V. Adwaith; T. W. Clark; Peter Domokos

Wigner Research Centre for Physics

Cold atoms prepared in the volume of a high-finesse optical resonator [1] form a hybrid quantum system that can serve as an interface between photonic and atomic qubits. Bistability in the hyperfine ground state of atoms [2] is useful for quantum sensing applications, while hybridized states of light and matter will be exploited in future quantum technology applications.

We experimentally demonstrate [3] strong collective coupling of the atoms to the cavity vacuum field by linear scattering from a transverse drive.

Arranging the atoms in an incommensurate lattice, with respect to the

resonator mode, the scattering can be suppressed by destructive interference: resulting in a subradiant atomic array. We show however, that strong collective coupling leads to a drastic modification of the excitation spectrum, as evidenced by well-resolved vacuum Rabi splitting in the intensity of the fluctuations. Furthermore, we demonstrate a significant polarization rotation in the linear scattering off the sub-radiant array via Raman scattering induced by the strongly coupled vacuum field.

[1] D. Varga, B. Gábor, B. Sárközi, K.V. Adwaith, D. Nagy, A. Dombi, T.W. Clark, F.I.B. Williams, P. Domokos, A. Vukics: Loading atoms from a large magnetic trap to a small intra-cavity optical lattice, Phys. Lett. A **505**, 129444 (2024).

[2] B. Gábor, D. Nagy, A. Vukics, P. Domokos: Quantum bistability in the hyperfine ground state of atoms, Phys. Rev. Research **5**, L042038 (2023).

[3] B. Gábor, K. V. Adwaith, D. Varga, B. Sárközi, Á. Kurkó, A. Dombi, T. W. Clark, F. I. B. Williams, D. Nagy, A. Vukics, P. Domokos: Demonstration of strong coupling of a subradiant atom array to a cavity vacuum, arXiv:2408.17079 (2024).

#C76: Quantum technologies, quantum optics, cavity QED, quantum information

Landau polariton

Farokh Mivehvar

University of Innsbruck

In quantum mechanics, the energy spectrum of two-dimensional electrons pierced by a uniform magnetic field are quantized into discrete, equally spaced levels, known as Landau levels (LLs). When such a system is placed inside a high-Q optical cavity and coupled strongly to a quantized cavity mode, Landau levels are then dressed by photons and form hybrid light-matter states, which I coin the name "Landau-polariton" for them. In this presentation, I show the exotic properties of these Landau-polariton states.

#C77: Quantum technologies, quantum optics, cavity QED, quantum information

Building scalable quantum computers at Oxford Ionics

A. C. Hughes; C. J. Ballance; C. M. Löschnauer; C. Matthiesen; D. T. C. Allcock; J. Mosca Toba; M. A. Weber; M. Krstajic; M. Malinowski; R. Matt; R. Nourshargh; R. Srinivas; S. A. King; T. P. Harty

Oxford Ionics

Building useful quantum computers means making them better as well as bigger. At Oxford Ionics we do this by combining the precision of trapped-ion qubits with the scalability of microelectronics. We replace the lasers conventionally used to manipulate ion qubits with electronics integrated directly into trap chips, which allows us to reach world-leading gate fidelities in a highly scalable architecture. We will present our architecture for all-electronic quantum gates with trapped ions, validated in a prototype quantum processor, and highlight how we build scalable hardware for trapped-ion quantum computing.

#C78: Quantum technologies, quantum optics, cavity QED, quantum information

Dissipation dilution in 3D direct laser written mechanical resonators

Daniel Stachanow; Lukas Tenbrake; Florian Giefer; Sebastian Hofferberth; Hannes Pfeifer

Uni Bonn

Optomechanical platforms with high-quality mechanical and optical resonators have a wide application potential ranging from quantum limited sensing to long-lived storage of quantum information. Whilst exceptionally high-quality factors have been realized with structures in thin layers of dielectric or semiconducting materials, their geometries are limited by the capacity of lithographic fabrication. Recent developments in polymer-based 3D direct laser-written structures allow for new paradigms in manufacturing micromechanical resonators, but so far suffer from strong mechanical dissipation. Here, we showcase our recent progress on implementing and improving this platform. The losses impacting the mechanical Q-factor of the resonator in vacuum are dominated by intrinsic losses within the material such as friction and thermoelastic damping. These losses, however, can be heavily reduced by introducing strain on the membrane, leading to so-called dissipation dilution. This is done by adjusting the fabrication process and engineering the geometry of the resonator for optimized aspect ratios.

To quantify the results of our methods a scannable vacuum-integrated fiber cavity setup for probing high quality-factor mechanical resonators is used. We present the impact of shrinkage-induced strain on the mechanical Q-factor of polymeric bridge-like resonators. Additionally, we report the status of our current developments using post-fabrication treatment of applying oxygen-plasma to further optimize the surface properties and aspect ratios of the structures.

#C79: Quantum technologies, quantum optics, cavity QED, quantum information

Creating and observing the hexadecapole moment in the fluorescence signal of the 87Rb D1 line: theoretical computations

Arturs Mozers; Daniela Jermacane; Florian Gahbauer; Marcis Auzins

University of Latvia, Faculty of Science and Technology, Laser Centre

Atomic magnetometers with magneto-optical signals based on Zeeman effect can achieve high sensitivity and accuracy in low magnetic fields, where the Zeeman effect is linear. In magnetic fields that exceed the Earth's magnetic field (~ 0.5 G), the nonlinear Zeeman (NLZ) effect introduces errors in magnetic field measurements. The NLZ effect does not affect ^{87}Rb ground-state sublevels with total angular momentum $F_g = 2$ and magnetic quantum number $m_{F_g} = \pm 2$ even at high magnetic field values. Acosta et al. [1] created coherences between these two sublevels by modulating the frequency of an exciting laser at twice the Larmor frequency, creating hexadecapole ($m_F = \pm 4$) and quadrupole ($m_F = \pm 2$) moment in the angular momentum distribution of the ^{87}Rb atoms. To eliminate the quadrupole moment, which exhibits NLZ effect, the laser modulation's phase is shifted by π to destroy the quadrupole moment in such a way as to retain the hexadecapole moment. This specially prepared state was observed by measuring magnetic-field-dependent rotation of a linearly polarized laser beam that passes through the rubidium vapour. We plan to adapt

this technique to measure the hexadecapole moment influence on fluorescence signals and study the effect of relaxation on the signal amplitudes using a theoretical model. We will report on the progress of theoretical modelling and describe the experimental setup.

We thank the Latvian Council of Science for support under Project No. Lzp-2023/1-0173 "Novel approach to improving accuracy and sensitivity of atomic Rb magnetometers".

[1] V. M. Acosta et al., Opt. Express, 16, 11423 (2008)

#C80: Quantum technologies, quantum optics, cavity QED, quantum information

Four-wave mixing in chip-scale Rb vapor cells in continuous wave mode

Heleni Krelman; Ori Nefesh; Liron Stern

The Hebrew University of Jerusalem

Four-wave mixing (FWM) is a nonlinear optical process in which two (or three) interacting optical fields generate two (or one) new fields via the medium's nonlinearity of third order $\chi^{(3)}$. Alkali vapors, especially those of Rb and Cs, exhibit exceptionally high nonlinear optical responses. Under near-resonant conditions, the third-order nonlinear susceptibility of these atomic vapors can exceed that of typical bulk nonlinear media by factors of 10^6 to 10^{10} .

Recently, silicon micromachining has revolutionized alkali vapor cell production, yielding chip-scale devices that are mass-producible, cost-effective, and multifunctional. These cells have already enabled high-performance atomic magnetometers [5,6], compact gradiometers [7], and chip-scale clocks [8,9], while offering exceptional miniaturization, stability, and seamless integration with on-chip photonic circuitry [10–12].

Traditionally, continuous-wave (CW) FWM has been realized in centimeter-scale vapor cells, where the extended interaction length facilitates efficient nonlinear conversion. In our work, we demonstrate for the first time that efficient CW FWM can be achieved in chip-scale micromachined Rb vapor cells, marking a significant step toward compact nonlinear optical platforms.

We employed resonant four-wave mixing (FWM) in millimeter-scale rubidium vapor cells to generate continuous-wave coherent emission at both blue and mid-infrared wavelengths. Under optimized conditions, the blue output reached $17 \mu\text{W}$ of continuous coherent power. Remarkably, replacing the anodically bonded Pyrex window with an anodically bonded silicon window enabled mid-infrared emission with powers up to 50 nW . We further characterized the temperature dependence and input-power scaling of the blue emission, confirming efficient nonlinear conversion within these compact vapor cells.

Incorporating injection-locking techniques can significantly boost the CBL and CMIRL output into the high-power regime, paving the way for compact, high-power sources suited for various applications. Our results underscore the potential of micromachined Rb FWM to serve as a compact, manufacturable platform for next-generation quantum devices.

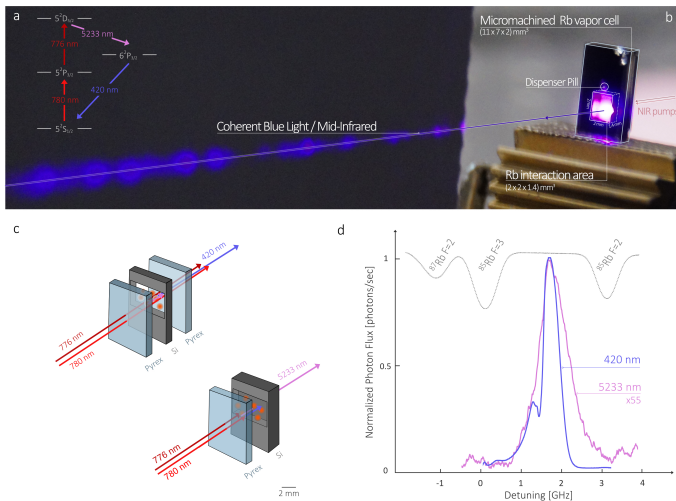


Fig.: Concept of continuous-wave four-wave mixing process in chip-scale Rb vapor cell. (a) Energy levels of ^{85}Rb illustrating the transitions involved in generating coherent blue light (CBL) and coherent mid-infrared light (CMIRL). The diagram highlights the excitation processes using the 780 nm and 776 nm lasers, leading to production of the 420 nm and 5.2 μm emissions. (b) Photo of generated light through FWM in micromachined Rb vapor cell. For clarity, the captions were added to the photo. By choosing the type of the cell, we may detect both CBL and CMIRL. (c) Schematic view on the chip-scale Rb cells used in this work. One has Pyrex backside (left), which absorbs 5.2 μm emission and transmits another three wavelengths involved in the process; another has Si backside (right) and transmits 5.2 μm emission only. (d) The number of photons per second as function of detuning of laser 780 nm for measured CBL (blue curve) and CMIRL (purple curve) with shown Rb reference (gray curve). Factor of 55 for CMIRL compared to CBL caused by losses.

References

- [1] S. Wang, J. Yuan, L. Wang, et al., "Measurement of the Kerr nonlinear refractive index of the Rb vapor based on an optical frequency comb using the z-scan method," *Opt. Express* 28, 38334–38342 (2020).
- [2] B. Ding, X. Yu, H. Lu, et al., "Third-order optical nonlinearity in silicon nitride films prepared using magnetron sputtering and application for optical bistability," *J. Appl. Phys.* 125, 113102 (2019).
- [3] K. Zhang, G. Böhm, and M. A. Belkin, "Kerr nonlinearity and group velocity dispersion of InGaAs/InP and GaAsSb/InP waveguides in the mid-infrared," *APL Photonics* 8, 066107 (2023).
- [4] R. Schiek, "Nonlinear refractive index in silica glass," *Opt. Mater. Express* 13, 066107 (2023).
- [5] K. Levi, A. Giat, L. Golan, et al., "Remote chip-scale quantum sensing of magnetic fields," *Opt. Quantum* 3, 84–92 (2025).
- [6] R. Mhaskar, S. Knappe, and J. Kitching, "A low-power, high-sensitivity micromachined optical magnetometer," *Appl. Phys. Lett.* 101, 241105 (2012).
- [7] J. Zhang and J. Shang, "Miniature quantum gradiometer using 3D interconnected atomic vapor cells," 2025 IEEE 38th Int. Conf. on Micro Electro Mech. Syst. (MEMS) pp. 589–591 (2025).
- [8] M. Pellaton, C. Affolderbach, Y. Pétremand, et al., "Study of laser-pumped double-resonance clock signals using a microfabricated cell," *Phys. Scr.* 2012, 014013 (2012).
- [9] S. Knappe, V. Shah, P. D. D. Schwindt, et al., "A microfabricated atomic clock," *Appl. Phys. Lett.* 85, 1460–1462 (2004).
- [10] H. Schmidt and A. R. Hawkins, "Electromagnetically induced transparency in alkali atoms integrated on a semiconductor chip," *Appl. Phys. Lett.* 86, 032106 (2005).
- [11] A. Goban, C.-L. Hung, S.-P. Yu, et al., "Atom-light interactions in photonic crystals," *Nat. Commun.* 5, 3808 (2014).
- [12] P. Londero, V. Venkataraman, A. R. Bhagwat, et al., "Ultralow-power four-wave mixing with Rb in a hollow-core photonic band-gap fiber," *Phys. Rev. Lett.* 103, 043602 (2009).

#C81: Quantum technologies, quantum optics, cavity QED, quantum information

Progress toward an atomic-beam continuous-wave superradiant laser

John Huckans¹; Benjamin Pasquiou²; Bruno Laburthe-Tolra²; Martin Robert-de-Saint-Vincent²; Yannis Pargoire²

¹ Commonwealth University of Pennsylvania / Sorbonne Paris Nord

² Université Sorbonne Paris Nord

Huckans J.^{†2}, Laburthe-Tolra B.¹, Pasquiou B.¹, Pargoire Y.¹, Robert-de-Saint-Vincent M.¹

¹Université Sorbonne Paris Nord, LPL, France

² Commonwealth University of Pennsylvania, Bloomsburg, PA USA

[†] jhuckans@commonwealthu.edu

We are building a continuous superradiant laser on the narrow (7.5kHz) intercombination line of ^{88}Sr using a cold, fast (10-100 m/s) atomic beam passing through the mode of a "bad" optical cavity. One of our goals is to study correlations that should arise between atoms, especially near the superradiant threshold.

Superradiant lasing is an emerging technology, which has been extensively studied both theoretically and experimentally. This light source can be used as a frequency reference. Fundamental quantum fluctuations of the collective atomic dipole set the ultimate laser linewidth, allowing it to be lower than the natural width of the transition and with a frequency only slightly dependent on fluctuations in the positions of the cavity mirrors. A continuous superradiant laser can therefore overcome many of the current limitations of atomic clocks.

In the case of a pulsed superradiant laser, the linewidth is defined as in (1, left). By contrast, the linewidth of a continuous-wave superradiant laser is defined as in (1, right). With our setup, designed to be a proof of principle of a continuous-wave superradiant laser in the bad-cavity regime, we expect to reach a linewidth of $\sim 700\text{Hz}$ (based on the 7.5kHz natural width). For this purpose, we choose a low ($C < 1$) single-atom cooperativity defined as $C = g^2/(\kappa\gamma)$, ($C = 0.211$ in our setup, with $g = 2\pi \times 31.54\text{kHz}$ the single-atom-cavity coupling term, $\gamma = 2\pi \times 7.5\text{kHz}$ the natural linewidth of the $^1\text{S}_0 \rightarrow ^3\text{P}_1$ transition, $\kappa = 2\pi \times 630\text{kHz}$ the cavity loss rate) and need a high collective cooperativity ($NC \gg 1$) with N the atom number inside the cavity.

$$\Delta\omega_{\text{Pulsed_SR}} = Ng^2/\kappa \quad \Delta\omega_{\text{Continuous_Wave_SR}} = 4g^2/\kappa \quad (1)$$

The dynamics of superradiance is described by the quantity Ng^2/κ . For superradiance to occur one needs a superradiance dynamics faster than the spontaneous emission, leading to $Ng^2/\kappa \gg \gamma$. The continuous-wave regime also requires a superradiance dynamics faster than the refreshing rate Γ_R of the cavity, leading to $Ng^2/\kappa \gg \Gamma_R$.

These conditions fix the minimum atom number to reach the superradiant emission threshold. For an atomic beam with a velocity of 100 m/s, this threshold is 80 atoms, a criterion we fulfill in our setup.

To achieve, control and characterize superradiance, we use a Zeeman slower to tune the atom velocity, thereby controlling the flux and the refreshing rate. Out of the Zeeman slower, we deflect the atoms toward the cavity. For this purpose, we use a moving molasses and have started to characterize its efficiency depending on the atoms' forward velocity. Then, we use SWAP (Sawtooth Wave Adiabatic Passage) Cooling² on the $^1\text{S}_0 \rightarrow ^3\text{P}_1$ transition to reach μK temperatures along the cavity axis. Finally, we have devised an adiabatic excitation scheme to be implemented just before the atoms reach the cavity, which we are currently testing.

Once our laser is emitting, we will characterize it with a beat note measurement and make photon quantum-correlation measurements. We will use the flexibility of our architecture to test different regimes such as having a distribution of velocities along the cavity axis that could lead to different collective dipoles³ and we will modify the cavity

to decrease the mirror reflectivity in order to reach a decreased laser linewidth.

1Bruno Laburthe-Tolra, Ziyad Amodjee, Benjamin Pasquiou and Martin Robert-de-Saint-Vincent, SciPost Phys Core 6, 015 (2023).

2John P. Bartolotta, Matthew A. Norcia, Julia R. K. Cline, James K. Thompson and Murray J. Holland, Phys. Rev. A 98, 023404 (2018).

3Simon B. Jäger, Haonan Liu, Athreya Shankar, John Cooper, Murray J. Holland, Phys. Rev. A 103, 013720 (2021).

#C82: Quantum technologies, quantum optics, cavity QED, quantum information

Observation of anomalous information scrambling in a Rydberg atom array

Xinhui Liang¹; Zonpei Yue¹; Yuxin Chao¹; Zhenxing Hua¹; Yige Lin²; Meng Khoon Tey¹; Li You¹

¹ Tsinghua University

² National Institute of Metrology of China

Study of information scrambling in a quantum many-body system is key to understanding the dynamics of thermalization and the evolution towards equilibrium. This work reports our experimental investigation into this topical subject by directly observing the out-of-time-order correlation (OTOC) function in a Rydberg atom array.

A key challenge in measuring the OTOC in an analog-digital hybrid circuit is the difficulty of implementing time-reversed evolution. We address this by leveraging the inherent constraints imposed by the strong van der Waals interactions in the Rydberg atom array system.

Our observations show that the scrambling dynamics for quantum many-body scar in a Rydberg atom array is anomalous, accompanied by a linear lightcone with a smaller valued butterfly velocity and persistent periodic oscillations inside, which differs from both thermal and many-body localized systems, and signifies an unusual breakdown of thermalization.

If time permits, I will briefly mention our another experiment on disorder-induced topology in a Rydberg atom array.

#C83: Quantum technologies, quantum optics, cavity QED, quantum information

An Apparatus for Controlling the Sr Clock Qubit

Marijn Venderbosch; Edgar Vredenburg; Gosia Kucharska; Jesús del Pozo Mellado; Max Festenstein; Rianne Lous; Rik Van Herk; Servaas Kokkelmans; Zhichao Guo

Eindhoven University of Technology

Arrays of optical tweezers loaded with neutral atoms have rapidly gained traction as a versatile and scalable architecture for quantum information processing. At Eindhoven University of Technology, we are developing a tweezer apparatus that allows control over single- and multi-qubit gates using the Sr clock qubit.

On the poster, we will present our recent experimental results of preparing single Sr atoms in our array of 5 x 5 optical tweezers. Spectroscopy measurements reveal an average tweezer depth of 0.51(2) mK and a standard deviation across of the array in the depth of 2.8%. Also shown are our first steps towards our two goals, which are site-resolved single-qubit operations using the ultranarrow 1S₀–3P₀ clock transition and implementing multi-qubit entangling gates via coherent excitation to Rydberg states using an ultraviolet laser.

Looking ahead, we aim to make this platform remotely accessible through the platform Quantum Inspire, opening the door for broader experimentation and algorithm development within the community.

PROGRAM

15th European Conference on Atoms, Molecules, and Photons



	Monday	Tuesday	Wednesday	Thursday	Friday			
8:00	Registration 08:00–08:30							
8:15								
8:30								
8:45	Welcome							
9:00	Plenary 1	Plenary 3	Plenary 5	Plenary 7	Plenary 9			
9:15	09:00–10:00	09:00–10:00	09:00–10:00	09:00–10:00	09:00–10:00			
9:30	Saal Tirol	Saal Tirol	Saal Tirol	Saal Tirol	Saal Tirol			
9:45	• Anne L' Huillier	• Tilman Pfau	• Jeffrey Hangst	• Jun Ye	• Mete Atatüre			
10:00	Coffee Break	Coffee Break	Coffee Break	Coffee Break	Coffee Break			
10:15	10:00–10:30	10:00–10:30	10:00–10:30	10:00–10:30	10:00–10:30			
10:30	Spectroscopy 1 Ultrafast 1 10:30–12:40 Saal Brüssel Saal Tirol • Miteva • Eckart • Nahon • Rohringer • Wcislo • Ayuso • Zhou • Tarallo • Chowdhury • Cassens	Large Systems 1 Quantum 2 Collisions 2 10:30–12:40 Saal Straßburg Saal Tirol Saal Brüssel • Nascimbene • Northup • Domaracka • Fennel • Garcia-Ripoll • Novotny • Mudrich • Thew • Zettergren • Tamames • Guizarro • Sinha-Roy • Bastian • Lopes • Buczolich	Plenary 6	Ultrafast 3 Spectroscopy 2 Ultracold 2 10:30–12:40 Saal Straßburg Saal Tirol Saal Brüssel • Gaarde • Patterson • Nic Chormaic • Boll • Ban • Bohn • Nandi • Hernandez-Garcia • Tarruell • Laliotis • Candas • Orsi • Gerlich • Both • Hofer	Quantum 4 Fundamental 2			
10:45			10:30–12:40		10:30–12:40	10:30–12:40		
11:00					• Dag Hanstorp			
11:15								
11:30								
11:45								
12:00								
12:15								
12:30								
12:45			Lunch Break		Lunch Break	Lunch Break	Lunch Break	Lunch Break
13:00			12:40–14:00		12:40–14:00	12:40–13:30	12:40–14:00	12:40–14:00
13:15						Excursions 13:30–18:00		
13:30								
13:45								
14:00	Plenary 2	Plenary 4	Plenary 8	Ultrafast 4 Spec. 3 + UC 4				
14:15	14:00–15:00	14:00–15:00	14:00–15:00	14:00–15:40				
14:30	Saal Tirol	Saal Tirol	Saal Tirol	Saal Brüssel Saal Tirol				
14:45	• Eleni Diamanti	• Beatriz Roldán Cuenya		• Marc Simon	• Tzallas • Fritzsche • Juzeliunas • Winter • Mirahmadi • Gėnėvriėz • Kristensen • Demes			
15:00	Coffee Break	Coffee Break		Coffee Break				
15:15	Poster Session A 15:15–17:00	Poster SessionB 15:15–17:00		Poster Session C 15:15–17:00				
15:30								
15:45					Closing Ceremony			
16:00					15:40–16:00			
16:15								
16:30								
16:45								
17:00	Collisions 1 Quantum 1	Fundamental 1 Ultracold 1		Ultracold 3 Quantum 3	Lab Tours			
17:15	17:00–18:40	Ultrafast 2		Collisions 3	17:00–19:00			
17:30	Saal Tirol Saal Brüssel	17:00–18:40		17:00–18:40				
17:45	• Willitsch • Rauschenbeutel • Balucani • Kaminer • Bogot • Ourjountsev • Yang • Liang	Saal Straßburg Saal Tirol Saal Brüssel • Mehlstäubler • Ni • Martin • Karr • Tomza • Remacle • Gerritsma • Tarbutt • Staudte		Saal Brüssel Saal Tirol Saal Straßburg • Pohl • Chu • Koch • Perrin • Poddubny • van de Meerakker • Marchetti • Vukics • Dernekhin • Marinelli • Fursa				
18:00								
18:15								
18:30								
18:45								
19:00			Welcome Reception 19:00–20:00		Conference Dinner 19:00–22:00			
19:15								
19:30								
19:45							Public Lecture by Rainer Blatt	
20:00							19:30–20:30	
20:15								
20:30								
20:45								
21:00								
21:15								
21:30								
21:45								
22:00								

SESSION LABELS

- Collisions:** Collisions of electrons, atoms, and molecules, highly charged ions, astrophysical processes

Spectroscopy: Atomic and molecular spectroscopy, photo-induced processes

Ultrafast: Femtosecond and attosecond physics, reaction dynamics, coherent control, strong f eld

Large Systems: Clusters, nanoparticles, biomolecules, surface interactions and self-assembly
- Ultracold:** Cold and ultracold atoms, molecules and ions, degenerate quantum gases, ultracold plasmas

Fundamental: Fundamental physics, precision measurements, atom interferometry and atomic clocks

Quantum: Quantum technologies, quantum optics, cavity QED, quantum information