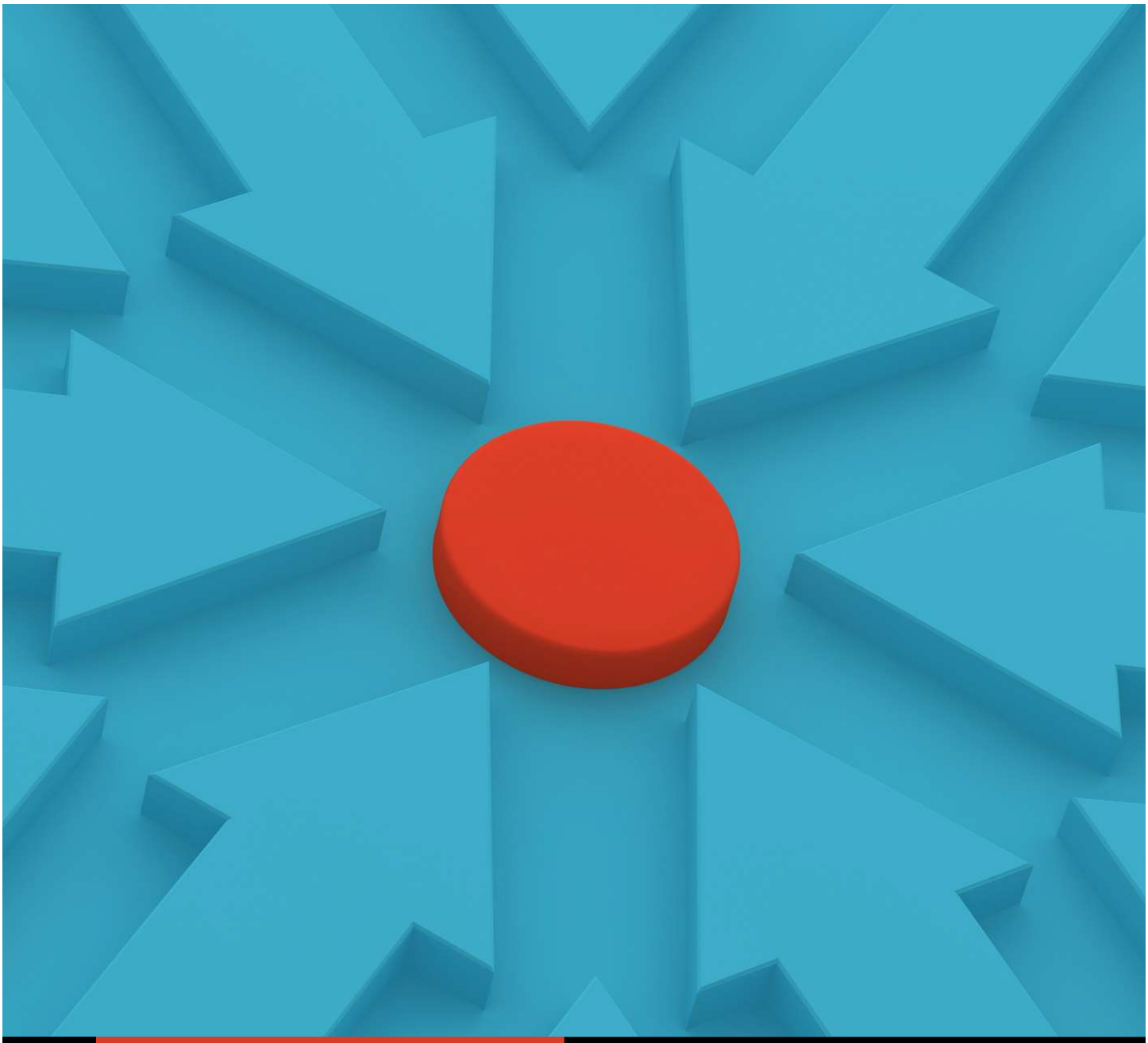
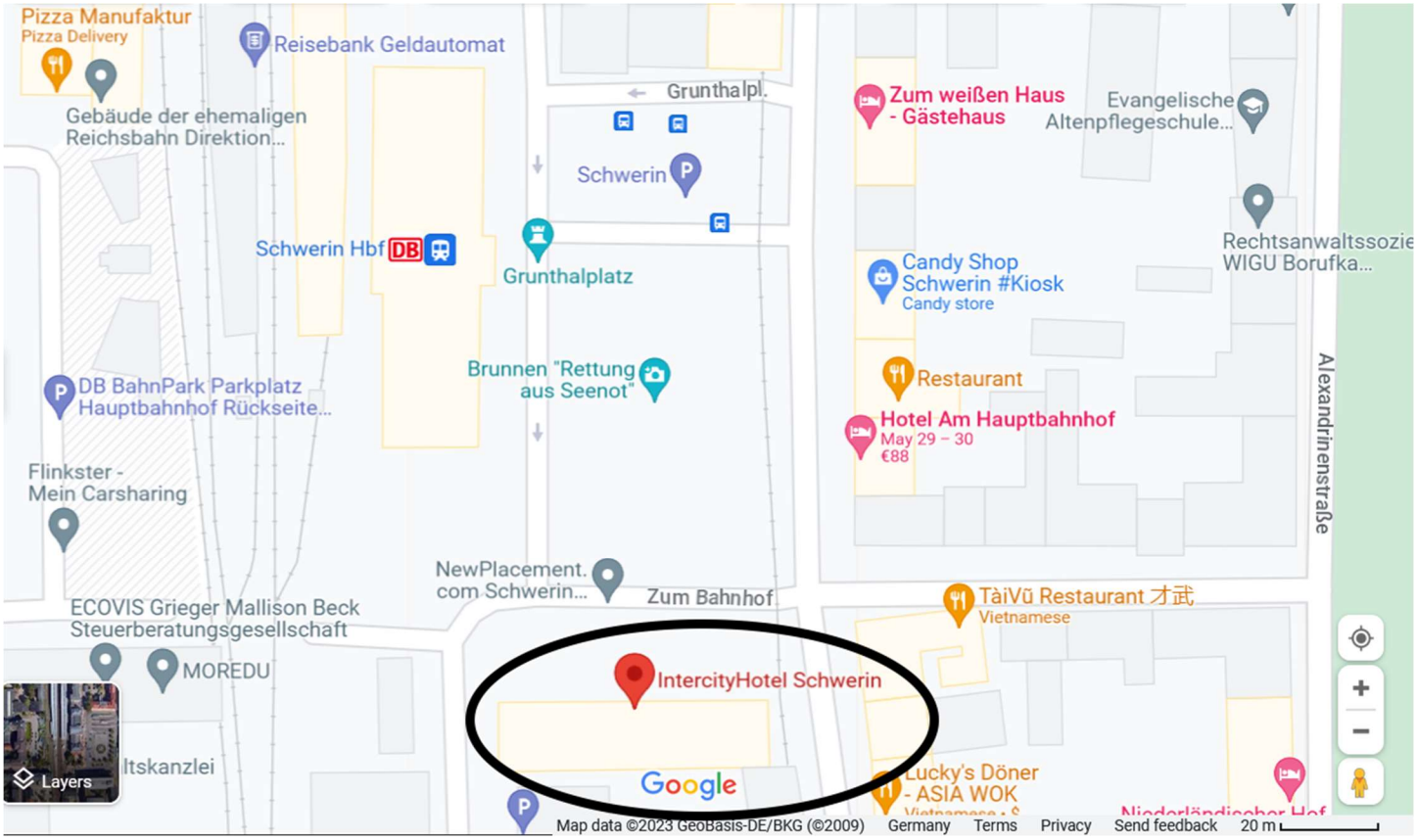


CUI SUMMER SCHOOL

5 TH OF JUNE – 9 TH OF JUNE 2023

aim.student-representatives@physnet.uni-hamburg.de



HOW TO REACH THE SCHOOL

The 2023 edition of the CUI summer school will take place at the InterCity Hotel Schwerin, in the beautiful city of Schwerin. The hotel is walking distance from the main station of Schwerin.

Please make use of the Deutschland ticket and travel by train, below a suggestion:

Ihre Reisedaten

Hinfahrt, Mo, 29.05.23

10:21	**Hamburg Hbf**	RE 1 (4309)
11:46	**Schwerin Hbf**	

Rückfahrt, Fr, 02.06.23

14:11	**Schwerin Hbf**	RE 1 (4310)
15:38	**Hamburg Hbf**	

	Monday		Tuesday		Wednesday		Thursday		Friday	
09:00-09:20	Travel	Travel	Pleanry Talk	John Travers Session 1	Pleanry Talk	Dorota Koziej Session 1	Pleanry Talk	Stefan Scheel Session 1	Student Talks Session 5	Jingxuan He
09:20-09:40										Prince Prabhu Rajaiah
09:40-10:00										Daniel Lengle
10:00-10:20										Julian Fiedler
10:20-10:40			Break	Coffee	Break	Coffee	Break	Coffee	Break	Coffee
10:40-11:00			Pleanry Talk	John Travers Session 2	Pleanry Talk	Dorota Koziej Session 2	Pleanry Talk	Stefan Scheel Session 2	CUI: AIM	Eileen Schwanold
11:00-11:20										CUI:AIM Diversity
11:20-11:40										
11:40-12:00										
12:20-14:00	Lunch									
14:00-14:20		Welcome	Student Talks Session 3	Sergey Ryabchuk	Free Afternoon	Free Afternoon	Transfer Agentur	Transfer Agentur ("Do I have product?")	Travel	Travel
14:20-14:40	Student Talks Session 1	Sarodi Jonak Dutta		Mukhtar Singh						
14:40-15:00		Felix Gerken		Jessica Harich						
15:00-15:20		Daniel Bosworth		Antonia Freibert						
15:20-15:40		Marcel Nathanael Kosch		Donika Imeri						
15:40-16:00	Break	Coffee	Break	Coffee			Break	Coffee		
16:00-16:20	Student Talks Session 2	Susanna Gevorgyan	Student Talks Session 4	Hamid Ahmadi Rashtabadi			Wired Sense	Wired Sense (Starting a Start-up)		
16:20-16:40		Helena Gleißner		Kai-Fu Wong						
16:40-17:00		Giovanni De Vecchi		Benoît Richard						
17:00-17:20		Niklas Witt		Sani Yusuf Harouna-Mayer						
17:20-17:30										
17:30-18:00	Poster Slam		Poster Slam				Poster Slam			
18:00-19:30	Dinner									
19:30-20:30	Poster		Poster		"Pub Quiz"		Poster			

Plenary Talks

Tues., Wed., Thur. 09:00 - 12:00

Nonlinear Optics in Gas-Filled Hollow-Core Fibres

John C. Travers
School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh, EH14 4AS, United Kingdom
j.travers@hw.ac.uk
https://lupo-lab.com

Hollow-core fibres, both with and without microstructure, provide a versatile platform for ultrafast nonlinear optics in gases, at high intensity over long interaction lengths, and have enabled a new class of optical light sources to be created [1, 2, 3]. Gas-filled hollow fibres can be transparent in regions of the electromagnetic spectrum ranging from X-rays to terahertz, and many gases, particularly the light noble gases, have ionisation energies significantly higher than those of solid-state materials. Combined, these properties mean that high optical pulse power and pulse energy can be transmitted and manipulated in hollow-core fibres over a wide spectral range. The fact that gases are compressible means that the material dispersion and nonlinearity of a gas-filled hollow fibre can be easily controlled during an experiment, allowing live dispersion and nonlinearity tuning. Furthermore, the fundamental character of the nonlinear response can be altered through the type of gas used and the role of plasma or Raman effects.

In these lectures, I will first review the fundamental properties of light-guidance in hollow-fibres, including the most important linear and nonlinear effects that occur, along with a brief history of their development. I will then explain how these properties can be exploited for sub-femtosecond pulse compression of near-infrared laser pulses using optical solitons [4, 5], for frequency up-conversion to the far-ultraviolet through either soliton dynamics [4, 9] or four-wave mixing processes [6, 7, 8], and for a new regime of broadband supercontinuum generation [10]. I will then proceed to describe out efforts to utilise these new light sources for both fundamental science, and for applications to industry and healthcare.

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[4] J. C. Travers et al., *High-energy pulse self-compression and ultraviolet generation through soliton dynamics in hollow capillary fibres*. Nat. Photonics **13**, 547–554 (2019)

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[6] F. Belli et al., *Strong and weak seeded four-wave mixing in stretched gas-filled hollow capillary fibers*. in *Ultrafast Optics 2019*, vol. 11370 (International Society for Optics and Photonics, 2019), pp. 1137001-46

[7] F. Belli et al., *Highly efficient deep UV generation by four-wave mixing in gas-filled hollow-core photonic crystal fiber*. Opt. Lett. **44**, 5509-5512 (2019)

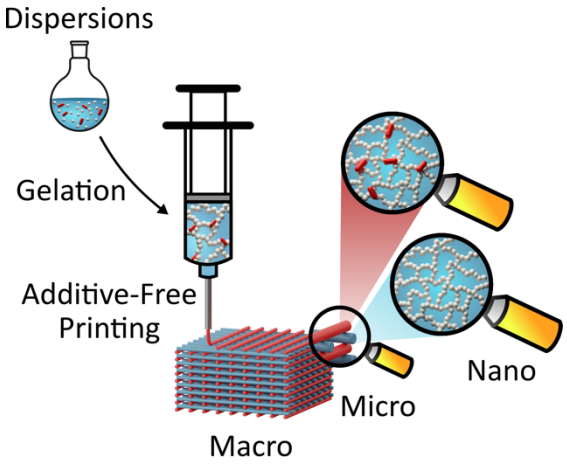
[8] A. Lekosiotis et al., *Generation of broadband circularly polarized deep-ultraviolet pulses in hollow capillary fibers*. Opt. Lett. **45**, 5648-5651 (2020)

[9] A. Lekosiotis et al., *Ultrafast circularly polarized pulses tunable from the vacuum to deep ultraviolet*. Opt. Lett. **46**, 4057-4060 (2021)

[10] S.-F. Gao et al., *From Raman Frequency Combs to Supercontinuum Generation in Nitrogen-Filled Hollow-Core Anti-Resonant Fiber*. Laser & Photonics Reviews, **16**, 2100426 (2022)

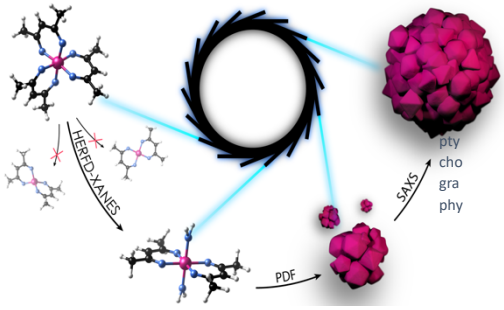
Complex materials – bridging the length scales in solution

Prof. Dorota Koziej



Over the past years we have developed various approaches to fabricate materials with sophisticated chemical and structural complexity. We have focused on synthesis in non-aqueous solution since this approach is not limited to one particular class of materials. Thus, it gives us flexibility to tailor the composition and properties of materials in respect to the application, for examples carbon dioxide sensors and photo-electrochemical devices.

First, I will discuss general approaches to transfer the unique properties of nanoparticles to macroscale, with emphasize on 3D-ink jet printing developed in our group. [1-2]



Then, I will present how X-ray synchrotron methods, far from merely providing new tools, are extending the ways we study, understand and design such complex structures. A combination of spectroscopic, scattering and microscopic X-ray methods and rapid data acquisition help to uncover the complex chemical world behind the synthesis of functional materials. It gives complementary information about chemical reaction in solution and nucleation, growth and crystal phase transition of nanoparticles. Moreover, on the selected examples, I will discuss how the possibility to select with high-energy resolution the incident and emission hard X-ray energies offers unprecedented site selectivity and give access to determine structure – function relationship of photo-, electroactive materials and devices. Finally, will discuss the advantages and the pitfalls of the synchrotron methods for in situ and operando studies. [3-5]

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Rydberg physics with semiconductor excitons

Stefan Scheel[1]

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Rydberg atoms, i.e. atoms that have been promoted to an electronic state with very large principal quantum number *n*, have some extraordinary properties compared to their ground-state counterparts. For example, their large dipole polarisability leads to giant van der Waals interactions [1]. The result is a strong shift in the energy levels of Rydberg atoms in close proximity, leading to the effect of Rydberg blockade in which the resonant excitation of a Rydberg atom is blocked in the presence of another Rydberg atom.
Recently, a completely different platform has begun to be explored in which Rydberg physics can be investigated. We have shown that Rydberg excitations can also be studied in the semiconductor cuprous oxide (Cu_2O) [2]. There, the objects under investigation are excitons — quasiparticle bound states that are formed by the Coulomb interaction between an electron and a hole. In the 2014 experiment, exciton bound states with principal quantum numbers up to n=25 have been observed, corresponding to an exciton wavefunction extending over 2μm.
In my lectures, I will introduce the notion of giant (van der Waals) interactions as applied to Rydberg atoms, and discuss some of their consequences and immediate applications in precision sensing, quantum information processing and quantum simulation. I will then explain the similiarities and differences between atomic and semiconductor-based Rydberg systems, including the concept of quantum defects in excitonic systems [3], the effects of broken rotational symmetry on dipole selection rules [4], and the influence of nanoplasmas on the Rydberg excitation spectrum [5]. The interplay between plasma and Rydberg interactions [6] is currently being resolved using pump-probe spectroscopy [7]. I will finally discuss the latest developments that concentrate on nanostructured materials [8] rather than bulk crystals that pave the way to compact miniaturized devices in which one can explore strongly interacting exciton-polaritons on a chip.

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Student Talks

Session 1

Monday 14:00 - 15:40

Self-assembly of colloidal nanoparticles: finding emergent properties in ordered structures?

Sarodi Jonak, Juan Jesus, Florian Schulz, Wolfgang J. Parak

Center for Hybrid Nanostructures (CHyN), Universität Hamburg, Germany

Nature has predominantly utilized the concept of self-assembly resulting in highly complex and functional structures such as pearl nacre [1]. The field of self-assembly of nanoparticles has moved from just forming two- and three-dimensional structures to focusing on the synthesis of new materials with tunable electrical, optical, and mechanical properties [2,3]. Hence, there is an ongoing quest in finding new interesting structures and physical properties from a very fundamental point of view, prioritizing rather well-defined, sophisticated, than large-scale structures. However, there are certain issues to be taken care of e.g., reproducibility, long-range periodic order, and truly emergent properties arising from the super-crystal formation can only be observed in a handful of systems. Recent experimental approaches with state-of-the-art electron microscopy, X-ray diffraction and scattering have helped in attaining a detailed picture of NP self-assembly processes and their structures. Further benefits are expected to arise from the design of the next-generation synchrotron radiation sources. We have been successful in assembling AuNPs of varying sizes into crystalline superlattices up to >0.01 mm^2 for monolayers and also larger crystalline multilayers with interparticle gaps in the range of 1-6 nm which led to the formation of new polaritonic excitations [4]. Furthermore, we have extended the protocol to additional nanoparticle systems. In this regard, we recently tried self-assembling PdNP@PSSH at the liquid-liquid interface. In order to understand the dynamics of the self-assembly of our systems, we are also exploring computational modeling using a general-purpose simulation toolkit, namely HOOMD-blue [5]. The increase in the number of highly functional self-assembled systems, and the emergence of fascinating new collective properties open new doors in both consumer and industrial space.

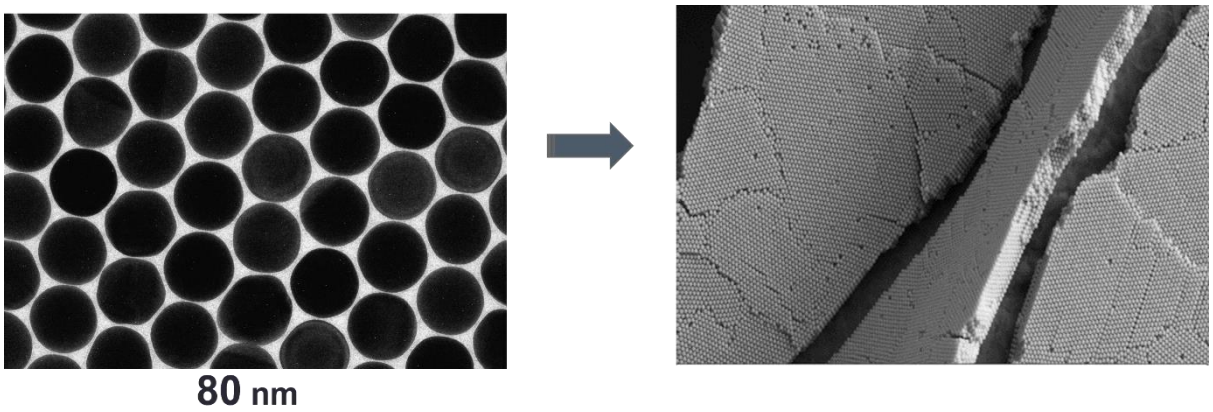

Figure. TEM and SEM micrographs of gold nanoparticle crystals consisting 80 nm gold nanoparticles.

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Large Degenerate Eigenspaces in Heisenberg Models from a Graphical Construction

Felix Gerken and Thore Posske

I. Institut für Theoretische Physik, Universität Hamburg, Germany and

The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

Strongly degenerate eigenspaces are an exciting phenomenon in spin glasses, spin ice, and topologically-degenerate quantum systems. We demonstrate how to construct models for one of the most prominent representatives of many-body systems which is partially amenable to exact solutions, the XXZ Heisenberg model. Starting with quantum spins attached to the vertices of an arbitrary graph, we reverse engineer XXZ models, also with on-site magnetic fields, that support simple product states as eigenstates. We derive sufficient conditions for product states to be eigenstates and show that the graphical representation of these rules is reminiscent of Kirchhoff's laws for electrical circuits. The graphical rules imply a construction procedure for a yet unknown class of potentially strongly degenerate spin models. For some of these models, the product eigenstates turn out to span a large degenerate eigenspace whose dimension scales exponentially with the number of spins. The singular nature of these eigenspaces hints at an intriguing connection between lattice topology, degeneracy and entanglement.

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[1] F. Gerken and T. Posske, Large degenerate eigenspaces in Heisenberg models from a graphical construction (in preparation).

Exciting trapped atoms with dragged potentials

Daniel Bosworth, Maxim Pyzh, Peter Schmelcher

We study the out-of-equilibrium dynamics of a single atom confined in a 1D harmonic trap triggered by dragging an external long-range potential through the system. The symmetry-breaking nature of the time-dependent potential leads to the emergence of trap-induced shape resonances (TISR) between adjacent eigenstates in the atom's effective potential. We propose to exploit the TISR to selectively excite the atom into higher vibrational states of the harmonic trap by controlling the speed at which the potential moves through the system. To this end, we consider two protocols: the first aims to maintain adiabaticity at critical points in the atom's dynamics, whereas the second relies on tunnelling in an asymmetric double-well potential. Our protocols, ranging from 1 ms to 1 s in duration, achieve high-fidelity excitations of the atom into pure vibrational states and superpositions thereof. Overall, our study highlights the significance of TISR in controlling and manipulating atom dynamics and offers intuitive protocols for achieving desired excitations.

Quantum gas magnifier for sub-lattice-resolved imaging of 3D quantum systems

Imaging is central to gaining microscopic insight into physical systems, and new microscopy methods have always led to the discovery of new phenomena and a deeper understanding of them. Ultracold atoms in optical lattices provide a versatile quantum simulation platform with a high degree of control over the system's parameters. Despite having lattice constants on the order of 1 micrometer, orders of magnitude above solid-state crystal structures, resolving the real space density distribution of the atoms in the lattice is still technologically very demanding. I will present an imaging approach where matter wave optics magnifies the density distribution before standard optical imaging, allowing 2D sub-lattice-spacing resolution in 3D systems[1]. By combining the site-resolved imaging with magnetic resonance techniques for local addressing of individual lattice sites, this gives full accessibility to 2D local information and manipulation in 3D systems. The sub-lattice resolution is demonstrated via quench dynamics within the lattice sites. With the single-site access, we can perform precision thermometry of Bose–Einstein condensates in optical lattices. We use the method to study out-of-equilibrium dynamics and identify an emerging density-wave, which spontaneously breaks the discrete translational symmetry of the system[2]. The method opens the path for spatially resolved studies of new quantum many-body regimes, including exotic lattice geometries or sub-wavelength lattices.

[1] Asteria et al., Nature **599**, 571-575 (2021)

[2] Zahn et al., PRX **12**, 021014 (2022)

Student Talks

Session 2

Monday 16:00 - 17:20

Structural dynamics of Tau protein and its condensates

Susanna Gevorgyan[1,2], *Prince Rajaiah Prabhu*[1,2], *Hévila Brognaro*[2], *Christian Betzel*[1,2]

[1] The Hamburg Centre for Ultrafast Imaging (CUI), University of Hamburg, Luruper Chaussee 149, 22761, Hamburg, Germany

[2] Institute of Biochemistry and Molecular Biology, Laboratory for Structural Biology of Infection and Inflammation, University of Hamburg, c/o DESY, Notkestrasse 85, Build. 22A, 22607 Hamburg, Germany

A recent breakthrough in studying the liquid-liquid phase separation (LLPS) phenomenon revealed that it is a fundamental mechanism underlying the formation and function of various membrane-less organelles and biomolecular condensates. In light of the association of LLPS with various pathological conditions, such as viral infections, cancer, and neurodegeneration, it is particularly interesting for research.

Tau is an intrinsically disordered protein implicated in Alzheimer's disease and other tauopathies. Its asymmetric charge distribution and strong interaction with polyanions enable it to phase separate. In this context, we examine the assembly and evolution of Tau protein's biomolecular condensates under various physicochemical conditions using advanced dynamic light scattering (DLS/DDLS) and complementary techniques. Recent results showing the sensitivity of selected biomolecular condensates to ionic strength variations and temperature gradients will be presented.

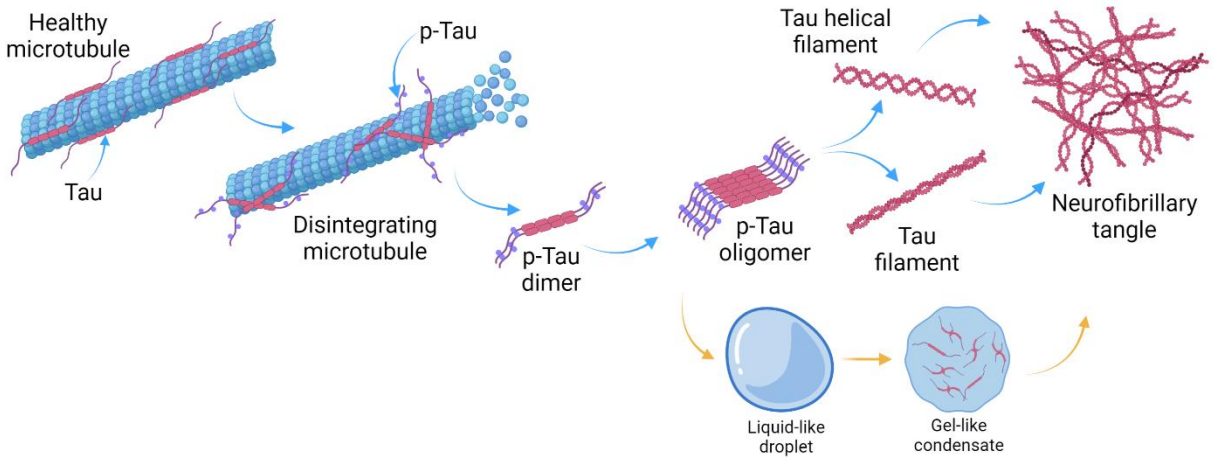

Figure 1. Tau protein phase separation and neurofibrillary tangle formation

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Time Resolved Photoemission Study of the Charge Transfer Dynamics in Rutile TiO_2(110) for CO Photooxidation to CO_2

Helena Gleißner [1,2,3], Michael Wagstaffe [2], Lukas Wenthaus [4], Simon Chung [2], Steffen Palutke [4], Siarhei Dziarzhytski [4], Dmytro Kutnyakhov [4], Michael Heber [4], Günter Brenner [4], Harald Redlin [4], Heshmat Noei [1,2], Andreas Stierle [1,2,3]

[1] The Hamburg Centre for Ultrafast Imaging, Hamburg, Germany

[2] Center for X-ray and Nano Science (CXNS), Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

[3] Fachbereich Physik Universität Hamburg, Hamburg, Germany

[4] Deutsches Elektronen-Synchrotron (DESY), Hamburg, Germany

Photocatalysts as TiO_2 are promising materials for harvesting solar light. Comparing the kinetics of photocatalytic reactions, anatase is the more active polymorph of TiO_2 compared to rutile. Still, the differences in the underlying dynamics for the oxidation of CO to CO_2 are not understood. In a pump-probe experiment at the free electron laser in Hamburg (FLASH) we gained insight into the ultrafast charge transfer on rutile TiO_2(110) during CO oxidation to CO_2. Pumped with a 770 nm optical laser and probed with 643 eV FEL soft x-rays we monitored the changes in the O 1s and Ti 2p core levels on a picosecond timescale using time-resolved photoemission spectroscopy. We find that oxygen gets activated and reacts with CO to CO_2 within 1 ps after the laser excitation. A complementary study found that the CO oxidation on anatase TiO_2(101) takes place between 1.2 and 2.8 ps after irradiation with an ultrashort laser pulse. [1]

[1] Wagstaffe, M. et al. ACS Catal. 10, 13650–13658 (2020).

Abstract ID : **12**

Search for the Ultrafast Meissner Effect in Driven YBa2Cu3O6.48

Content

Photo-excitation at terahertz and mid-infrared frequencies has emerged as a new way to manipulate functionalities in quantum materials, in some cases creating non-equilibrium phases that have no equilibrium analogue.
In cuprate high-Tc superconductors, resonant excitation of certain lattice vibrations has been shown to induce transient terahertz reflectivity features suggestive of nonequilibrium superconductivity above the critical temperature Tc.
Exploring these exotic states beyond their conductivity, as extracted from their terahertz reflectivity, is crucial to shed light on their complex nature.
In particular, a defining feature of equilibrium superconductors consists in their expulsion of static external magnetic fields: the Meissner effect.
To probe this effect in the short lived light-induced state, we use optical magnetometry, a technique which enables measurements of the magnetic field inside a laser-driven material on picosecond time scales, based on probing the Faraday effect in an adjacent crystal.
Here, we report preliminary findings from optical magnetometry measurements that suggest the presence of a Meissner effect in a photo excited sample of underdoped YBCO above its critical temperature.

Primary authors: Dr BUZZI, Michele (MPSD MPI Hamburg); Prof. CAVALLERI, Andrea (MPSD MPI Hamburg); FAVA, Sebastian (MPSD (Max-Planck-Forschungsgruppe)); Dr GEBERT, Thomas (MPSD MPI Hamburg); JOTZU, Gregor (MPSD); DE VECCHI, Giovanni (CFEL-QCM (Quantum Condensed Matter Dynamics Group))

Presenter: DE VECCHI, Giovanni (CFEL-QCM (Quantum Condensed Matter Dynamics Group))

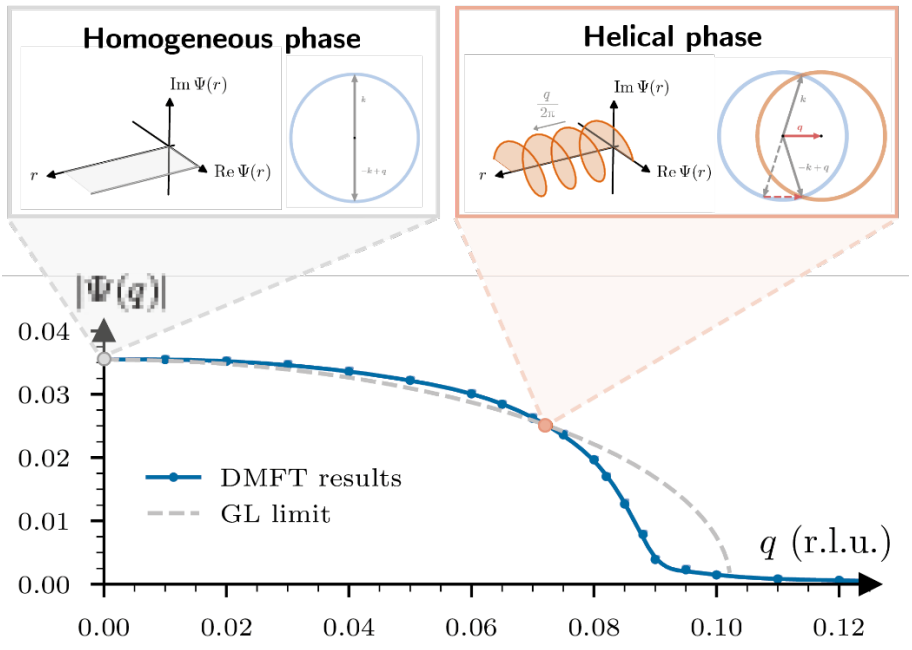
Submitted by **DE VECCHI, Giovanni** on **Friday, 19 May 2023**

Coherence and pairing fluctuations in strongly correlated superconductors

Niklas Witt, *Yusuke Nomura, Sergey Brener, Ryotaro Arita, Alexander I. Lichtenstein, Tim O. Wehling*

The fundamental properties of superfluids and superconductors are determined by the spatial coherence of the macroscopic condensate. Its fluctuations are pivotal to supercurrent flow, the functionality of superconducting nanostructures, and the response superconducting matter shows to magnetic fields. Central to a theoretical description is the coherence length which sets the relevant length scales of fluctuation effects. While a microscopic link is well established in weak-coupling BCS theory and Eliashberg-theory, it is a generally unknown quantity in strongly correlated superconductors where spatiotemporal fluctuations influence the critical temperature [1] and might underlie light-induced enhancement of superconductivity [2].
Here, we establish a link to directly calculate the coherence length as well as depairing currents and critical fields for superconductors with strong electron correlations from microscopic theories and first principles. We illustrate with the example of Alkali-doped fullerides (A_3C_{60}) how proximity of superconducting and Mott-localized states impact superconducting coherence, pairing localization, and critical temperature. In our analysis, we identify two different superconducting regimes that might be tunable in experiment (e.g. external laser fields).

[1] Emery & Kivelson, Nature 374 (1995)
[2] Fausti et al., Science 331 (2011); Mitrano et al., Nature 530 (2016)



Student Talks

Session 3

Tuesday 14:00 - 15:40

Mapping the UV-induced dynamics of CH_3I with 5 fs resolution

Sergey Ryabchuk[1,2], Lorenzo Colaizzi[2,3], Erik P. Månsson[3], Krishna Saraswathula[3], Jesús González-Vázquez[4], Vincent Wanie[3], Andrea Trabattoni[3,5], Fernando Martin[4,6,7] and Francesca Calegari [1,2,3]

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Methyl iodide (CH_3I) has become a benchmark molecule for time-resolved ultraviolet (UV) spectroscopy [1]. The lowest-lying states of the molecule, forming the A-band, are accessible by single UV photon absorption in the energy range between 4.1-5.4 eV [2]. The prompt dissociation of the band is accompanied by a passage through a conical intersection (CI) along the C–I reaction coordinate. The CI crossing is expected to be reached in ~ 10-20 fs timescale, imposing difficulties in being observed experimentally [3, 4].
In this work, we use our recently developed light source delivering broadband UV pulses with central energy of 4.9 eV [5] to populate the A-band. The UV-induced dissociative dynamics were probed via multiphoton ionization induced by ultrashort near-infrared (NIR) pulses with 5-fs time resolution.

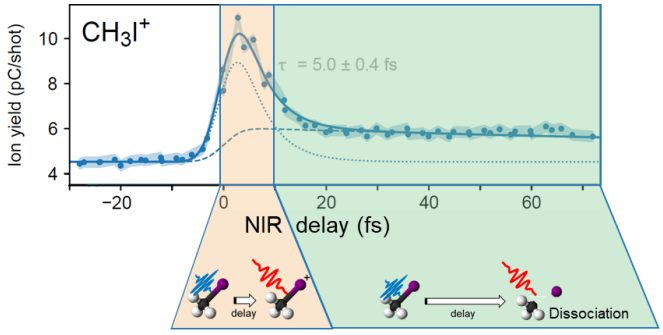

Fig. 1 The parent ion time-dependent signal with a schematic illustration for manipulating the CH_3I dissociation probability.

The extreme time resolution provided by the use of few-cycle pulses allows us to benchmark a full-dimensional classical trajectory simulation that has been used to predict the neutral evolution through the formation of CH_3I^+, CH_3^+ and I^+ cations. In turn, the benchmarked theoretical model allows us to extract the time to reach the conical intersection and analyze its dependence on the excitation energy. Notably, a 5-fs decay time observed in the time-dependent yield of the parent ion reveals that the probability for the UV-induced cleavage of the C-I bond can be manipulated by adjusting the delay of the NIR probe pulse in a narrow time window after excitation (illustrated in Fig. 1) [6], therefore offering a new control scheme for the photoprotection of the molecule against dissociation.

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UV and thermal-energy chemical dynamics of solvated (bio)molecular complex systems

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We present the investigation of ultrafast chemical dynamics induced by UV and thermal-energy excitation in micro-solvated (bio)molecular complexes. The interaction between small (bio)molecules and their solvents serves as a model system for studying the interactions between proteins and their environment [1]. Here we give focus to the hydrogen-bonded cluster, indole-water [2,3], which is important due to indole's role as the chromophore of tryptophan, the strongest near UV absorber in proteins.

The experimental setup contains a molecular beam and the electrostatic deflector to produce a pure gas-phase sample of indole-water [3]. To study the photo-induced dissociation dynamics, we conducted a UV-IR pump-probe experiment, wherein we excited the system to the electronic $\pi\pi^*$ state using 270 nm light. The dissociation dynamics of the micro-solvated system were monitored using strong-field ionization by 1.3 μm wavelength light from a femtosecond pulsed laser, tracking the time-dependent ion signals of the indole-water clusters, as well as the individual indole and water ions. The observed major time constants were attributed to the initial interconversion to the optically dark $\pi\sigma^*$ state, followed by the return to the ground state.

For studying the thermal-energy chemical dynamics, we employed a mid-IR pump to excite the N-H, and C-H vibrational modes, which induced dynamics between the indole and water moieties. By using this mid-IR pump, we aimed to mimic the thermal-energy excitation of (bio)molecular systems observed in nature. We monitored the dynamics of the system using the same 1.3 μm ionizing laser pulses, enabling us to draw comparisons between the dynamics of thermally-electronically-excited systems.

Furthermore, the study aims to utilize laser-induced electron diffraction (LIED) [4] to probe the thermally-excited molecular system and acquire structural information about the system with atomic resolution. LIED is a rapidly evolving technique that can be utilized in pump-probe experiments to study the structural changes of molecular systems on Femto- to picosecond timescales. Our group has initiated work on LIED and has already determined the geometry and bond distances of the OCS molecule, which were extracted from our measurement with a precision better than ±5 pm, in full agreement with the known structure of ground-state OCS [5]. We intend to expand upon these outcomes and conduct time-resolved studies of thermal-energy excited indole-water molecules.

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Residue Size Dependency of the In-cage Geminate Recombination Dynamics of the Biologically Relevant Disulfide Moiety after UV-cleavage investigated by time resolved X-ray Spectroscopy

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The tertiary structure of proteins is stabilized by disulfide bonds formed from two spatially adjacent L-cysteinyl residues. But these disulfide bridges are prone to UV radiation damage with potentially adverse effects to the stability of a protein's tertiary structure. We demonstrated the use of time resolved X-ray spectroscopy (TRXAS) - uniquely useful for the identification of photoproducts with high chemical specificity due to probing the sulfur core-level transitions - at the sulfur K edge to observe the UV photochemistry of small organosulfur compounds in nonpolar solvent environments [2-3]. From these models we moved to the natural amino acid dimer L-Cystine [1] and the tripeptide Glutathione (GSSG) in aqueous solution to understand the photochemistry under physiological conditions with increasing chain length. In the latest step of this bottom-up approach, we have first exciting insights into the UV-photochemistry of the disulfide bridges within the protein hen egg white Lysozyme (Fig.1).

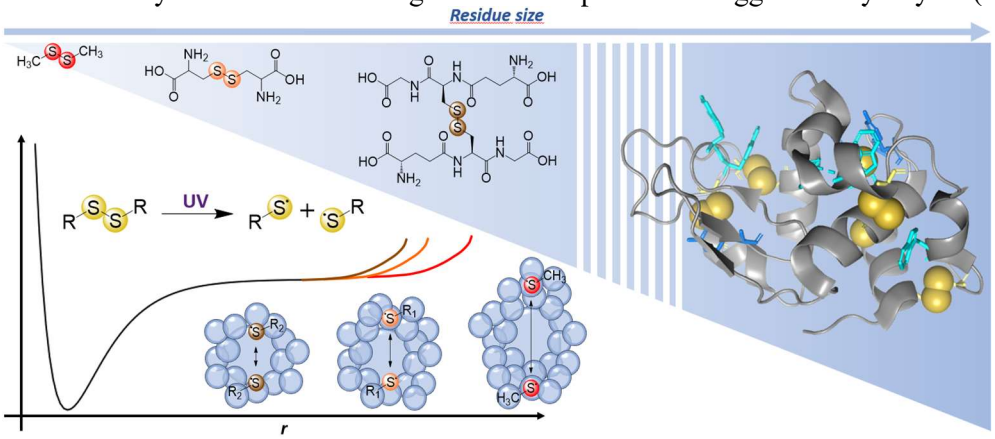

Fig. 1 Top: Aliphatic disulfides with increasing residue size: dimethyl disulfide (DMDS, red S atoms), L-cystine (orange S atoms), glutathione disulfide (brown S atoms) and the protein Lysozyme, which has four disulfide bonds. Bottom: Breaking of the disulfide bond using UV light. Schematic on the influence of residue size on photoproduct expulsion and recombination dynamics within the solvent cage.

We find that upon UV irradiation, apliphatic disulfides immediately undergo S-S bond cleavage, leading to the formation of two identical thiyl radicals, followed by fast geminate recombination indicating a very effective recombination process for thiyl radicals to the ground state. This process is only possible in condensed phases and its speed increases with chain length. Our results show that L-Cystine already captures the essence of the ultrafast photochemistry of the disulfide bridge, but that the size of the residue adjacent to the disulfide bonds has a strong influence on the immediate recombination dynamics of the photoproducts.

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On the Importance of Core-excited State Dynamics in Time-resolved X-ray Spectroscopy of Pyrazine

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Recent developments of short-pulse X-ray sources have enabled the extension of ultrafast pump-probe techniques into the X-ray domain allowing to measure not only equilibrium X-ray spectra but also to track dynamical processes in transient species. The combination of element-specific core-level probing with femtosecond time resolution greatly extended the ability to observe photoinduced electronic and structural changes. Due to the complex nature of detecting structural dynamics on ultrafast time scales, detailed theoretical studies are required to link the spectroscopic observables to the underlying dynamics and thereby access the high information content of ultrafast X-ray spectra. A large influence of nuclear dynamics can be expected in nonlinear spectroscopy which requires a time-dependent framework that is able to describe non-adiabatic phenomena.

I will present time-resolved X-ray spectroscopy simulations of pyrazine at the nitrogen K-edge including wavepacket dynamics in both, the valence- and core-excited state manifolds. The validity of the widely used short-time (or Lorentzian) approximation which neglects the nuclear dynamics following the X-ray interrogation will be discussed. Furthermore, the impact of an explicit description of the external electric field will be demonstrated where the effect of the pulse duration on the observed photo-triggered wavepacket dynamics is explicitly calculated.

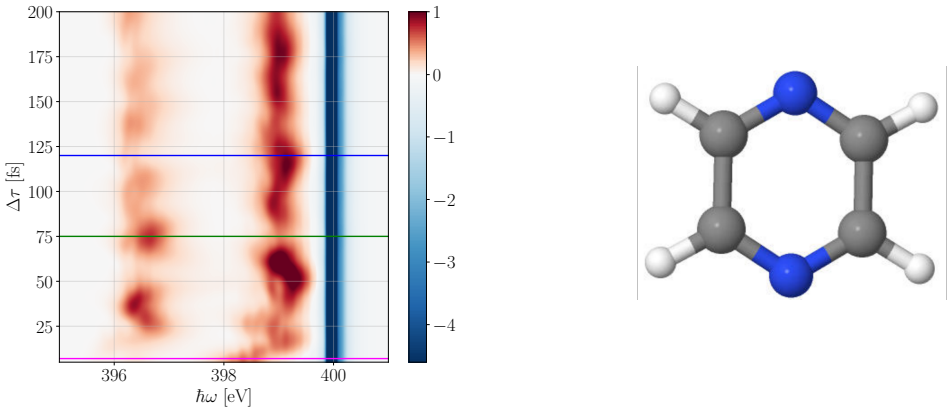

Fig. 1 Computed differential absorption spectra for time delays between 0 fs and 200 fs (left) of pyrazine (right) at the nitrogen K-edge.

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Toward High Fidelity Quantum Networks - Silicon Vacancy Centers in Diamond

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Quantum networks combine high security with the ability to scale up the number of qubits, which is essential for large-scale quantum information processing. These networks have nodes that store quantum data. Entanglement can be used to connect these nodes and enable quantum communication. Silicon-vacancy (SiV) color centers in diamond are promising candidates of optically coupled quantum processors. These solid-state emitters provide an effective optical interface and exhibit protective inversion symmetry. As a result, it is feasible to incorporate them into nanophotonic structures. The entanglement between spin- and photonic qubits can be generated using this approach. Coherent interactions between nuclear spins and the SiV require ultra-low temperatures and strong currents that simultaneously generate radio-frequency fields. Here we present a platform integrating superconducting coils with nanophotonic structures for operation at millikelvin temperatures.

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Figures

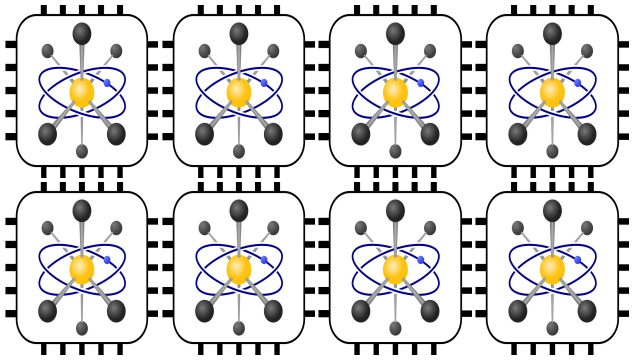

Figure 1: Schematic of a quantum network with SiV-centers as nodes. Connecting the color centers are photons distributing the entanglement.

Student Talks

Session 4

Tuesday 16:00 - 17:20

Abstract ID : **9**

Consequences of providing equal opportunity for the fast and slow parts of chirped ultrashort pulses

Content

The adaptive approach of using Cherenkov soliton radiation in optical fibers, which is widely known as resonant dispersive wave emission (or non-solitonic radiation, or rogue waves in optical fibers), allows for the spectro-temporal modulation of ultrashort pulses and nonlinear frequency conversion. Our experiment involved manipulating near-infrared ultra-broadband pulses close to the zero-dispersion wavelength, which allowed both the slow and fast parts of chirped pulses to remain synchronized. This led to the different frequency components of a broadband pulse overlapping in time with themselves, facilitating a frequency wave mixing condition that causes the generation of new frequencies.

In general, in a medium with a normal dispersion regime, shorter wavelengths of a broadband pulse propagate slower than longer wavelengths, while this is reversed in an anomalous dispersion regime, and in this case, the different frequencies of a broadband pulse can not have a chance of time overlap. But under certain circumstances, a pulse can partially propagate in an anomalous dispersion while the rest propagates in a normal regime. This causes the pulse to fold in the time domain, allowing its wings of spectrum to overlap temporally with themselves, which allows it to transfer energy to new frequencies.

If a broadband pulse propagates in two different dispersion regimes, higher-order dispersion terms will dominate. These higher-order dispersions perturb a soliton and disperse energy from the main pulse, which causes an optical pulse to radiate at a new frequency that depends on a particular phase-matching condition.

Driven by a spectrally broadened Ti:sapphire laser compressed down to 7 fs, we experimentally demonstrate a compact ultraviolet source emitting tunable ultraviolet non-solitonic radiation in a one meter argon-filled hollow cappilary fiber with a radius of 70 microns. This novel approach offers a promising alternative to traditional ultraviolet sources. The use of a hollow cappilary fiber allows for efficient nonlinear interactions between the laser pulse and the gas medium, resulting in the generation of high-quality ultraviolet radiation. By tuning the dispersion, we can control the frequency of the emitted radiation, making this source highly versatile and adaptable to a wide range of applications. Furthermore, the compact size of this system makes it ideal for use in field experiments or other situations where space is limited. Overall, our results demonstrate the potential of this new approach for generating high-quality ultraviolet radiation in a compact and cost-effective manner.

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Presenter: AHMADI RASHTABADI, Hamid (UNI/EXP (Uni Hamburg, Institut fur Experimentalphysik))

Submitted by **AHMADI RASHTABADI, Hamid** on **Thursday, 18 May 2023**

Far-field petahertz sampling of plasmonic fields

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Plasmon excitation in nanosystems allows for extreme light confinement beyond the diffraction limit, therefore enabling a number of new applications in photonics, energy harvesting and biology. In this context, it is key to obtain a realtime characterization of the onset from the plasmonic field and its ultrafast dephasing dynamics. Tunnel ionization with a perturbation for the time-domain observation of an electric field, short TIPTOE, is a recent established technique allowing for the optical sampling of ultrashort laser pulses based on strong field ionization. The main requirement of this technique is the use of a sufficiently short gate to induce ionization in a gas target. Subsequently, this ionization is modulated by a weaker pulse to be sampled. With this method it is possible to characterize arbitrary electric fields as long as ionization by the weak pulse itself does not occur [1,2]. Here, we implement TIPTOE for the optical sampling of linear plasmonic fields measured in the far-field regime.

In our experiment, sub 5 fs pulses with a central wavelength of 780 nm are exciting plasmonic gold nanoparticles embedded on a fused silica substrate, the transmitted beam is then sent into a TIPTOE setup for the optical field sampling. Two different shapes for plasmonic samples have been used, namely spherical and rod-shaped particles. While the latter sample displays a broadband plasmonic resonance, i.e. the longitudinal localized surface plasmon resonance (L-LSPR), covering a major part of the few-cycle spectrum, the plasmonic resonance of the spherical particles is located outside the exciting broadband pulse bandwidth.

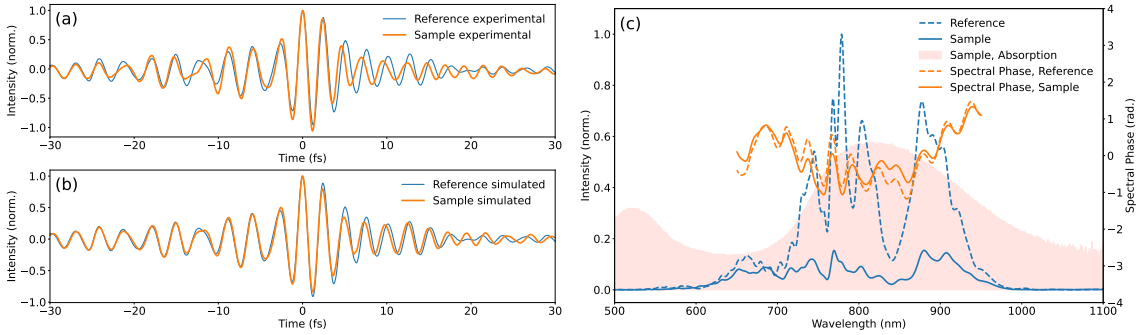

Fig. 1 Normalized (a) measured TIPTOE traces and (b) simulated traces for the electric field after interaction with the plasmonic sample. As reference the input field is depicted in blue, which was also used as the input field for the FDTD simulation. (c) Retrieved spectrum (blue) and spectral phase (orange) via FFT for the plasmonic sample. The retrieved spectra were normalized to the reference. The dashed lines display the retrieved spectra and spectral phase of the input field respectively. The shaded area displays the absorption spectra of the plasmonic nanorods.

The measured traces for the in-resonance plasmonic samples strongly differ from the few-cycle input field, with a large deviation window in the trailing edge of the laser pulse and within a 20 fs delay range. The retrieved spectrum exhibits the expected strong reduction of intensity due to large absorption induced by the L-LSPR and remarkable effects in the spectral phase, which displays a crossing in the region of the plasmon resonance. These effects are not observed with the off-resonance excited particles, therefore confirming that a strong signature of the plasmonic excitation persist in the far-field. The obtained results were compared with theory using finite difference time domain (FDTD) simulations, where the detection of the electric field is performed after the plasmonic sample to mimic the far-field conditions of the experiment. The simulations reproduce the same deviations observed in the experiment well, therefore confirming that a measurement in the far-field still carries crucial information on the excited plasmonic field. These results not only pave the way to realtime observation of plasmonic fields from arbitrary samples on the petahertz scale, but also opens interesting perspectives in the engineering of the spectral phase of ultrashort laser pulses.

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Excruciating technicalities necessary to keep the dream of Coulomb Explosion Imaging alive

Benoît Richard

We love molecules and we love ultra-short and ultra-intense x-ray pulses. It is an impossible love, however, as making both meet in an experiment makes the former violently break apart in a process called Coulomb explosion. As with any breakup, there is much to learn here. The strategy is to measure the momenta of the atomic fragments in coincidence, a feat that has been experimentally demonstrated[1, 2].

Now the theoretical question that remains is how much and what exactly can we learn from this Coulomb explosion tragedy? Maybe it is not much, and then the dream of using Coulomb Explosion for imaging is broken, like so many dreams, and should be abandoned. I am however a believer, and in this talk, I will explain our approach to keep the dream alive. It aims to reconstruct the full multivariate distribution of momenta and link it to the ground state vibrational modes of the exploded molecule. It represents a first step at mapping the measurable distribution of asymptotic ion momenta to the distribution of geometries of the molecule. A full distribution was never imaged directly before, as most methods focus on reconstructing the average geometries, keeping away from the beautiful but slightly nightmarish world of multivariate distributions. The general concept, mapping what we can measure to what was going on just before the explosion, seems straightforward at first glance, but the devil is in the details.

Being friends with the devil, I will use the opportunity to have you trapped in a room with me for 15 minutes to tell you all about the technicalities required to make this project comply with our objective. I will plant them in your brain like painful little needles that could, by chance, hit a nerve activating interest. It is not too unlikely as many subjects will be discussed, including statistical methods, data processing, and automatic differentiation.

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Title: In situ Total X-ray Scattering and X-ray Absorption Spectroscopy of ultrasmall copper palladium nitride nanoparticles

Abstract: Transition metal nitride (TMN) nanoparticles are an interesting class of materials because of a variety of promising application in catalysis, energy storage or conversion. Yet, they are relatively unexplored today, which is due to their instability and tendency to oxidize in ambient condition. Further their synthesis is challenging. The main origin is the unreactive nature of common nitrogen reagents which necessitates high-temperature and/or high-pressure synthesis.
To give a comprehensive picture of the reaction we combine Totals X-ray Scattering (TXS), Small Angel X-ray Scattering (SAXS) and X-ray Absorption Near Edge Structure (XANES) spectroscopy on the in situ synthesis of copper palladium nitride which yields small nanoparticles at relatively low temperature and no pressure. XANES spectroscopy probes the electronic structure of copper and palladium throughout the reaction showing the precursor decomposition, formation of intermediates and final nanoparticles. TXS and the Pair Distribution Function (PDF) further shows the nucleation, growth and phase changes during the reaction. Finally, SAXS allows to monitor the size distribution and shape evolution during the reaction.

Student Talks

Session 5

Friday 09:00 - 10:20

Selection and control of cryogenically-cooled (bio)nanoparticle beams with external fields

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Unraveling the elementary steps of biological processes and chemical reactions has been a long-time goal. By using x-ray single-particle diffractive imaging, we can investigate the three-dimensional molecular structure of individual nanoparticles at atomic resolution through reconstructing a series of two-dimensional diffraction patterns [1].

However, because of the typically low signal-to-noise ratio, this requires the collection of a large amount of diffraction patterns. Since every intercepted particle is destroyed by the intense x-ray pulse, a new and preferably identical sample particle has to be delivered to every pulse. Here, we present an approach to prepare dense beams of cryo-cooled nanoparticles and macromolecules with buffer-gas cell cooling and aerodynamic focusing techniques [2-3].

Besides, we developed several control mechanisms with external fields at room temperature. For example, realizing a stream of pure, identical particles with electric field [4], and aligning the particles' arbitrary orientation in space by applying optical field (ns-laser induced alignment). Envisioned future experiments plan to make use of our cryogenic nanoparticle cooling setup together with efficient field-control to achieve a very high degree of alignment for shock-frozen proteins and, in turn, subnanometer resolution in single particle x-ray imaging.

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Dynamics of Tau condensate modulation by suramin applying time-resolved dynamic light scattering

Prince Rajaiah Prabhu[1,2*], Janine Hochmair[3], Hévila Brognaro[1], Susanna Gevorgyan[1,2], Maximilian Franck[3], Robin Schubert[6], Kristina Lorenzen[6], SelinYazici[1], Eckhard Mandelkow[4,5], Susanne Wegmann[3], Christian Betzel[1,2,*],

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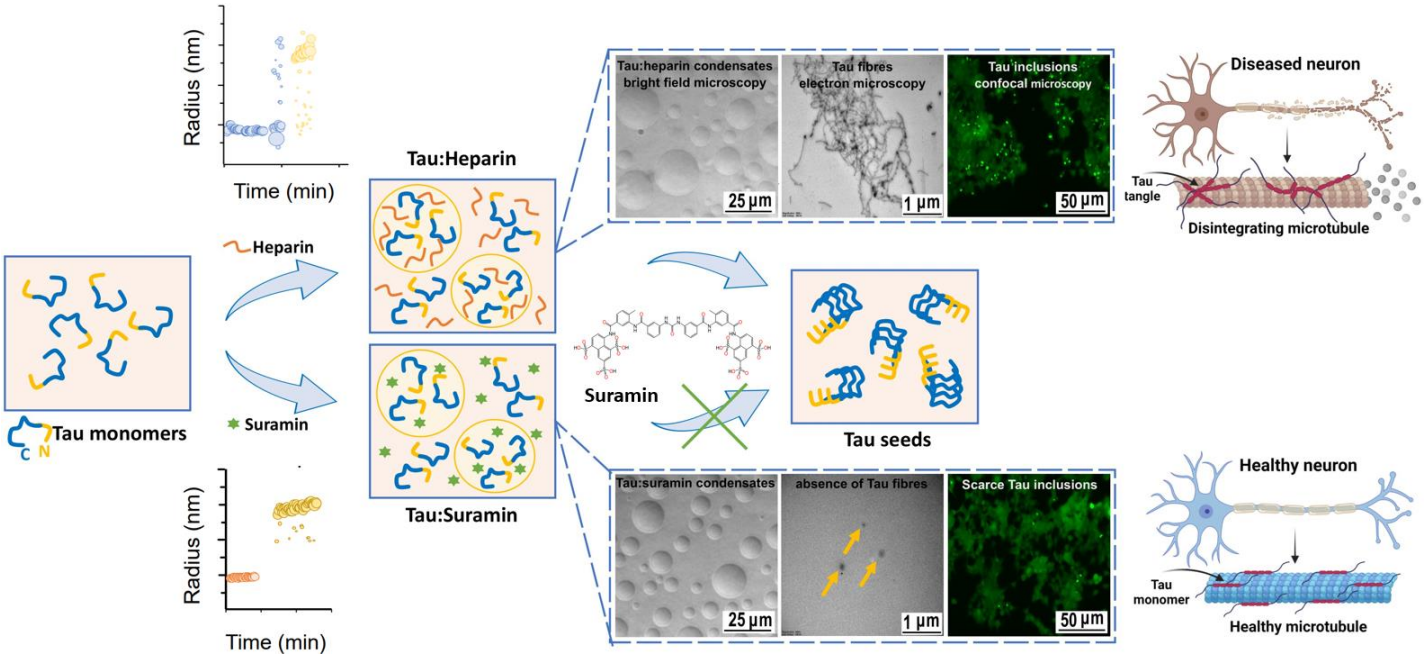
Abstract

Tau plays a key role in the hall mark sign of neurofibrillary tangles observed in Alzheimer's disease (AD). From our earlier studies[1,2], we showed that Tau forms biomolecular condensates and over time has potential to develop pathological aggregation seeding potential in a HEK model[1]. We extended this study[3] to identify the role of potential polyanionic small molecules and found suramin, a parasitic repurposed drug to induce liquid-liquid phase separation (LLPS) of Tau. We applied time resolved dynamic light scattering experiments (trDLS) to understand intermolecular electrostatic interactions between Tau and suramin. We also applied light and electron microscopy confirm the dimensions of Tau:suramin condensates. Our studies also show that Tau:suramin condensates do not seed Tau aggregation in a HEK cell model for Tau aggregation. Applying electron microscopy, we further confirmed the mitigation of heparin-induced tau fibril formation by the modulation of suramin during extended incubation[3]. These findings from our study indicate that suramin like anionic small molecules can electrostatically modulate Tau condensation without causing pathological aggregation and provides an innovative therapeutic strategy to intervene aberrant Tau phase separation. We also propose that applying trDLS to study the effect of polyanionic compounds on protein condensation is more appropriate for investigating these processes at an early dynamic stage of condensate evolution.



References :

1 Hochmair, J. *et al.* Molecular crowding and RNA synergize to promote phase separation, microtubule interaction, and seeding of Tau condensates. *EMBO J*, e108882 (2022). https://doi.org:10.15252/embj.2021108882

2 Wegmann, S. *et al.* Tau protein liquid-liquid phase separation can initiate tau aggregation. *EMBO J* **37** (2018). https://doi.org:10.15252/embj.201798049

3 Prince Rajaiah Prabhu, J. H., Hévila Brognaro, Susanna Gevorgyan, Maximilian Franck, Robin Schubert, Kristina Lorenzen, SelinYazici, Eckhard Mandelkow, Susanne Wegmann, Christian Betzel. Initiation and modulation of Tau protein phase separation by the drug suramin. *Scientifc Reports* (2023). https:// DOI: 10.1038/s41598-023-29846-9

Ex-situ monitoring of the cation exchange on individual semiconductor nanowires

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[2]The Hamburg Center for Ultrafast Imaging, Hamburg, Germany

The properties of nanostructures are largely determined by their material composition and their geometry. Chemical cation-exchange reactions allow for a controlled change of the elemental composition within a nanostructure while its geometry is preserved.

We investigate individual semiconducting CdS or CdSe nanowires after successive cation-exchange steps with silver. For this purpose, nanowire field-effect transistors are fabricated via optical lithography, as sketched in figure 1b. These devices are characterized by atomic force microscopy to obtain crucial parameters as nanowire diameter and channel length. Then the cation exchange is performed by submerging the device in a silver-nitrate solution. By precisely timing the duration in the solution, the reaction progress and thus the exchange degree can be controlled. Transport measurements reveal a change in conductivity (see figure 1c), charge-carrier concentration, and mobility. Confocal photoluminescence spectroscopy on the other hand gives insight into the material composition and the bandgap of the materials. Figure 1a shows that the CdS near band edge emission decreases as the exchange progresses.

We prove that the cation exchange can be monitored and investigated with a minimum of interference in the reaction. Nanowires with carefully adjusted elemental composition, and thus adjusted optoelectronic properties, could possibly find a way into electrical devices such as sensors, transistors or batteries.

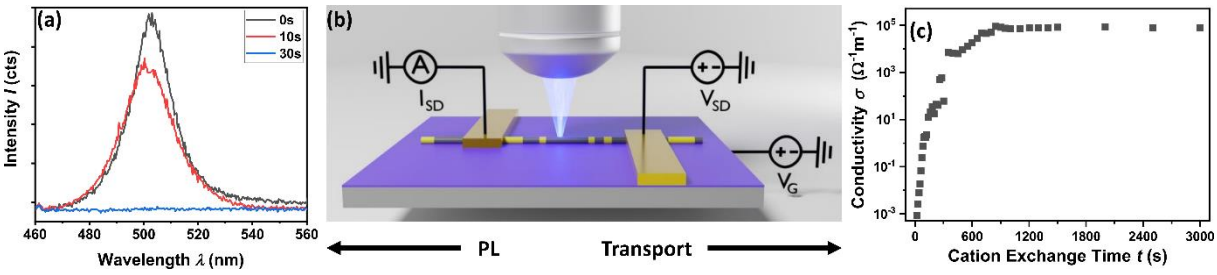

Figure 1: (a) Photoluminescence spectra of a CdS nanowire after a certain exchange duration. (b) Schematic overview of the investigation on a single nanowire field-effect transitor. (c) Conductivity evolution of a CdSe nanowire with ongoing exchange.

A velocity map imaging spectrometer and ion microscope for ultracold atoms

Julian Fiedler[1,2], Jette Heyer[1,2], Mario Großmann[1,2], Amir Khan[2], Klaus Sengstock[1,2], Markus Drescher[1,2], Juliette Simonet[1,2], Philipp Wessels-Staarmann[1,2]

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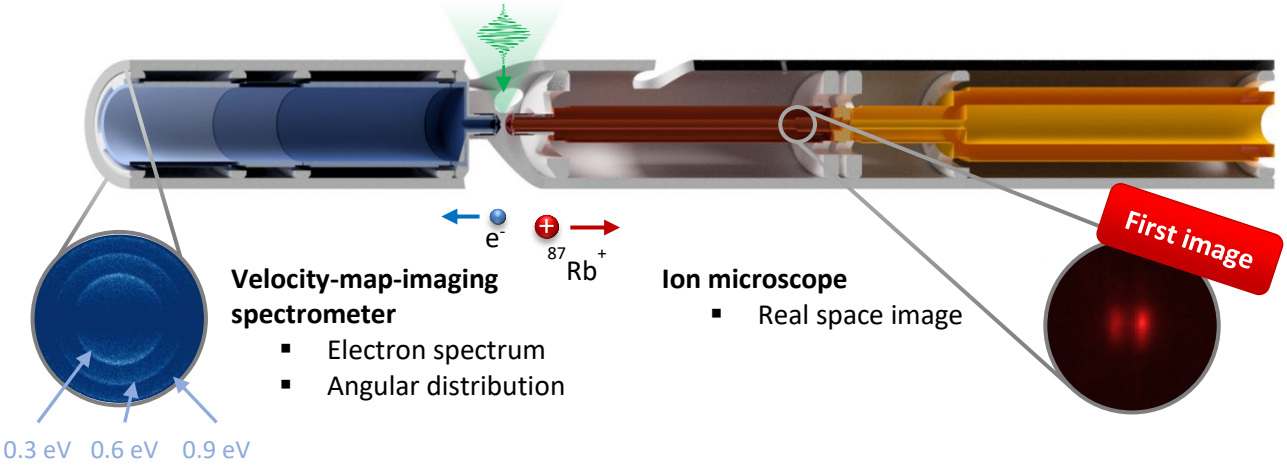
Ultrashort laser pulses provide pathways for manipulating atomic quantum gases on femtosecond timescales. By focusing a single femtosecond laser pulse onto a Bose-Einstein condensate, a controlled number of charge carriers can be created, forming hybrid systems ranging from few ion-atoms-, to complex many body systems.

For probing such systems, a coincidence detection unit consisting of a high-resolution ion microscope and a Velocity-Map-Imaging spectrometer is under construction. The new detection unit will allow the simultaneous measurement of the spatial distribution of ions with a simulated spatial resolution of 100 nm and the momentum distribution of electrons with a relative resolution of 10% over six orders of magnitude. Moreover, the pulsed extraction of both ions and electrons grants access to the dynamics of hybrid atom-ion systems or bound states with long-range interactions.



Posters

Monday, Tuesday & Thursday

Poster Slam 17:30 - 18:00

Poster Session 19:30 - 20:30

	Name	Poster Title
Monday	Emanuele Rossi	Theory of preparation of wave-packets by means of XFEL attosecond pulses
	Giovanni De Vecchi	Search for the Ultrafast Meissner effect in driven underdoped YBCO
	Sunil Kumar Mahato	Thin Film Diamond Nano-photonics and its quantum Application
	Laurin Georg Lang	Supercharging Mutations in Binary Nanocage Assemblies + X
	Jim Skulte	Quantum rotation sensor with real-time readout based on an atom-cavity system
	Marty Rogers	Nuclear Magnetic Resonance for Protein Structural Studies
	Eva Paprotzki	heory for Time-Resolved X-Ray Spectroscopy on Correlated Electrons
	Jan Lukas Dresselhaus	Towards high resolution X-ray imaging using MLLs
	Rosmaelle Kouemo	Subcycle Resolved X-ray imaging of Laser Driving Quantum Materials
	Mei Bai	Quantum dissipative theory of EXAFS in polar solvents.
	Marvin Skiba	Polyelectrolte Capsule assisted delivery of anticarcenogenicselinium drug
Tuesday	Tatiana Bezriadina	X-ray absorption by laser-driven system
	Josina Hahne	UV generation in gas in a differentially pumped chip
	Benoît Richard	Fun generalities about the prospects of Coulomb Explosion Imaging
	Daniel Bosworth	Effective quantum state transfer using dragged impurities
	Francesco Valiera	Electrons interacting in time: a noisy description
	Joseph Adelinia	On-Chip Ultrafast Transport Probe of Nonequilibrium Superconductivity
	Dimitris Triandafillidis	Emergence of order form proteins under nucleation
	Matthew Robinson	Imaging of Thermal-energy Dynamics
	Huan Zhao	femtosecond Dynamics of Ag29 nanoclusters by UV-Vis Spectroscopy
	Michaela Schneeberger	Using (ab-initio) MD-simulation to investigate (confined) aqueous solutions
	Lukas Haas	Laser-induced alignment of nanoparticles
	Rukan Nasri	Super Resolution Laser Assisted Detection of Molecules
	Nicolas Heimann	TBC
Thursday	Zeki Zeybek	Quantum Phases from Competing van der Waals and Dipole-Dipole Interactions of Rydberg Atoms
	André Becker	Non-equilibrium Dynamics of Few Trapped Fermions
	Felix Klein	Quantum state tomography of a nanomechanical resonator in a pulsed measurement protocol
	Meny Menashes	towards quantum Sr simulator using tweezer array
	Thies Plassmann	Towards quantum simulation with strontium atoms
	Jette Heyer	Many to few: From ultracold plasma to atom-ion hybrid systems
	Ioannis Ioannidis	Proximity superconductivity in atom by atom crafted quantum dots
	Marcel Herber	Bubble Printing of Ti3C2 MXene for Patterning Conductive and Plasmonic Nanostructures
	Michael Lau	Moving Antiferromagnetic Skyrmions with Spin Waves
	Alexander Wolff	Squeezed-Light-Enhanced Mass Photometry
	Alexandra Mozdzen	Two-dimensional Bose Gas with Tuneable Interaction Strength
	Shivani Kesarwani	Incorporation of organic dye in to gold nanoparticle superlattices and study it's excited state dynamics
	Aarathi Sathi Nair	Usingelectrosprayionizationandtandemmass spectrometrytostudystructureanddynamicsof biomolecules
	Suman Sanki	Magnet(4fsystem)-superconductorhybridsystem studiedbySTM/STS
	Daniel Lengle	Monitoring of the cation exchange in individual nanowires

Transfer Sessions

Thursday 14:00 - 17:20

From science to innovation:
How to found and operate a technology start-up?

Matthias Budden and Thomas Gebert

WiredSense

WiredSense GmbH, Luruper Hauptstr. 1, 22547 Hamburg

www.wiredsense.com

The start-up company WiredSense was founded out of experimental research as a part-time project next to our academic work in laser and solid-state physics. Initially, we developed a highly sensitive infrared- and terahertz (THz) detector as a research prototype for laser characterization and now sell it as a commercial product that has become the world's fastest pyroelectric THz detector. Based on this technology, we are currently bringing our mid-infrared spectrometer Sweeb from prototype-stage to the market. With this compact and cost-effective device, we build a cloud-based platform that enables chemical material analysis without a lab and within seconds and addresses a broader user range compared to the specialized THz detector.

We share our firsthand experience of founding and operating a hardware-based company in the electronic and optic sector and discuss the pros and cons of starting a company on a part-time basis. We review common obstacles we encountered, such as legal and financial challenges, and highlight the support and funding opportunities we received. Moreover, we present effective strategies and digital tools for product development and production that are particularly relevant (not only) for part-time founders.