OePG-CMD-JOINTMEETING 2026

75th Annual Meeting of the Austrian Physical Society

and

32nd Meeting of the Condensed Matter Division
of the European Physical Society

20 - 25 September 2026

University of Graz, Graz Center of Physics, Graz, Austria

Program & Abstracts

OePG Sections & CMD Mini-Colloquia

	Monday (21)	Tuesday (22)	Wednesday (23)	Thursday (24)	Friday (25)
	MORNING	MORNING	MORNING	MORNING	MORNING
08:30-09:00	Opening				
09:00-10:00	Plenary 1	Plenary 4	Plenary 7	Plenary 10	Plenary 13
	Riel	Bocquet	Pepper	Shapiro	Degerman
09:00-10:00	Plenary 2	Plenary 5	Plenary 8	Plenary 11	Plenary 14
	Sinova	Huber	Seddon	Gschwendtner	tba
10:00-10:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
10:30-12:30	Mini-Colloquia	Mini-Colloquia	Mini-Colloquia	Mini-Colloquia	Mini-Colloquia
	Excursions M11 M12/1 M14 M23/1 M03/1 M28/1 M04/1 M32 M10/1 M39/1	AwardCeremony M06/1 M19 M09 M23/2 M10/3 M28/2 M16 M29/1 M17/1	AWS/ERC FAKT/2 M21/1 M01 M25 M05/1 M27/1 M06/2 M30 M12/3 M37/2	OeAW M18/1 NESY/1 M21/3 PIN M26/2 FAKT/3 M27/3 M5/4 M31/1 M6/3 M37/3 M13/1 M38/1 M42/1	OGD/4 M29/5 COND4 M33/3 YM/3 M36 M05/3 M37/1 M13/3 M41 M15/2 M42/3
12:30-13:30	Break	Break	Break	Break	Closing Remarks
13:30-14:30	Posters (PS1)	Posters(PS1)	Posters(PS2) *OePG General Assembly*	Posters (PS2)	
	AFTERNOON	AFTERNOON	AFTERNOON	AFTERNOON	
14:30-15:30	Plenary 3	Plenary 6	Plenary 9	Plenary 12	
	Maurer	Coclite	Gull	Reichert	
14:30-15:00	Semi-Plenary 1	EurophysPrize	Semi-Plenary 3	Semi-Plenary 5	
	Geerts		Akrap	Juraschek	
15:00-15:30	Semi-Plenary 2		Semi-Plenary 4	Semi-Plenary 6	
	Kowalczyk		Giessen	Rotter	
15:30-16:00	Coffee break	Coffee break	Coffee break	Coffee break	
16:00-18:00	Mini-Colloquia	Mini-Colloquia	Mini-Colloquia	Mini-Colloquia	
	AKCP/1 M07/1 AMP M10/2 ENS M12/2 GEP M20/1 MBU M22/1 M03/2 M35 M04/2 M39/2	AKCP/2 M08 COND/1 M10/4 FAKT/1 M17/2 LHS M20/2 OGD/1 M22/2 M02/1 M29/2 M07/2 M34/2	COND/2 M21/2 OGD/2 M26/1 YM/1 M27/2 M02/2 M29/3 M05/2 M33/1 M07/3 M34/1 M12/4 M40	COND/3 M18/2 NESY/2 M24 OGD/3 M29/4 YM/2 M31/2 M02/3 M33/2 M05/5 M38/2 M13/2 M42/2 M15/1 M18/2	

Sunday (20)				
Registration and Reception 16:00-20:00		***OePG Board Meeting*** 18:00-19:30	**Public Talk** 18:30-19:30	**Conference Dinner** 18:30-22:00	

Poster Session PS1: AKCP AMP MBU M02 M03 M08 M09 M10 M11 M12 M19 M20 M23 M35

Poster Session PS2: COND FAKT NESY OGD YM M01 M05 M18 M24 M27 M29 M30 M33 M37 M42

Plenary Talks

Plenary 1 (Mon 21, 09:00-10:00)			
ID	Title	Speaker	Type
820	**tba**	Heike Riel	Plenary talk

Heike Riel (1)

(1) IBM Research Zürich, Switzerland

Plenary 2 (Mon 21, 09:00-10:00)			
43	**Unconventional Magnetism: the emergence of altermagnetism and beyond**	Jairo Sinova	Plenary talk

Jairo Sinova (1)

(1) Johannes Gutenberg University Mainz

Antiferromagnetic spintronics has been a very active research area of condensed matter in recent years. As we have learned how to manipulate collinear antiferromagnets actively and their emergent topology by means of new types of spin-orbit torques, a key problem remained: the inefficiency of relativistic mechanism. The necessity of relativistic effects to manipulate and detect Néel order arises from the spin degeneracy of collinear antiferromagnets in the non-relativistic limit – or at least it was thought. The discovery of d-wave magnetic order in momentum space motivated a closer look at the symmetry classification of collinear magnetic systems. This has emerged as the third basic collinear magnetic ordered phase of altermagnetism, which goes beyond ferromagnets and antiferromagnets. Altermagnets exhibit an unconventional spin-polarized d/g/i-wave band structure in reciprocal space, originating from the local sublattice anisotropies in direct space. This gives properties unique to altermagnets (e.g., the spin-splitter effect), while also having ferromagnetic (e.g., polarized currents) and antiferromagnetic (e.g., THz spin dynamics and zero net magnetization) characteristics useful for spintronics device functionalities. I will cover the basic introductory view to altermagnetism and its consequences to spintronics as well as new emerging exchange driven phenomena akin to spin-orbit coupling effects, such as p-wave magnetism, emerging from the basic concepts that gave rise to the discovery of altermagnetism.

Plenary 3 (Mon 21, 14:30-15:30)			
754	**Deus ex machina: Augmenting first principles theory with machine learning methods**	Reinhard Maurer	Plenary talk

Reinhard Maurer (1)

(1) University of Vienna

Atomistic simulation based on quantum mechanics (QM) is currently being revolutionized by machine-learning (ML) methods. Many existing approaches use ML to predict materials properties based on first principles reference data. This has enabled materials property prediction within vast compound spaces and high-dimensional parametrization of energy landscapes for the efficient simulation of measurable observables. However, as all properties derive from the electronic wave function, an ML model that can predict the wave function or the electronic Hamiltonian also has the potential to predict other properties. In this talk, I will explore ML approaches that deliver surrogate models of the electronic structure [1,2] to develop methods that use ML and QM in synergy. Using example systems from heterogeneous catalysis and organic electronics, I will discuss the challenges associated with encoding physical symmetries and invariance properties into linear and deep learning mappings of atomic configuration and composition onto electronic structure. Upon overcoming these challenges, integrated ML-QM methods within modern, modular software frameworks offer the combined benefits of data-driven parametrization and first-principles-based methods [3]. I will discuss several opportunities associated with building ML-augmented first principles methods, including Inverse Chemical Design based on ML-predicted electronic structure and the development of efficient and accurate surrogate models to study ultrafast dynamics in materials [4,5].

[1] C. Qian, V. Vitartas, J. Kermode, R. J. Maurer, npj Computational Materials (2026), in press, arXiv:2508.15108 (2026).
[2] L. Zhang et al., npj Computational Materials, 8 (2022) 158.
[3] P. Stishenko et al., J. Chem. Phys (2026), in press, DOI: https://doi.org/10.26434/chemrxiv-2025-xn2mp-v3
[4] M. Sachs, W. G. Stark, R. J. Maurer, C. Ortner, Mach. Learn.: Sci. Technol. 6 (2025), 015016.
[5] G. Meng et al., Phys. Rev. Lett. 133 (2024), 036203.

Plenary 4 (Tue 22, 09:00-10:00)			
78	**The Molecular Mechanics of Fluids**	Lyderic Bocquet	Plenary talk

Lyderic Bocquet (1)

(1) CNRS and Ecole Normale Supérieure, Paris, France

The emerging field of nanofluidics explores the molecular mechanics of fluids at the smallest scales. This realm of the "infinitely small in fluidics" is the frontier where the continuum of fluid dynamics meets the atomic nature of matter, and even its quantum nature. Observations unveil a cabinet of curiosities of singular properties, from frictionless flow to neuromorphic behaviors.
In this talk, I will discuss experimental and theoretical results that we obtained recently on the transport of water and ions in nanopores, both in 1D nanotubes and 2D channels obtained by van der Waals assembly. I will in particular focus on the emergence of hydro-electronic couplings, explaining the strange flows of water in carbon nanotubes. This opens new perspectives for nanoscale fluid transport, which I will illustrate on the phenomena of flow tunneling across walls, and (ion-free) hydro-electronic energy conversion.

Beyond the scientific intrigue, some of the singular nanoscale properties can be scaled up to develop innovations at the water-energy nexus. I will in particular discuss how this led to revived large-scale perspective for osmotic energy harvesting, as well as large-scale application for separation and desalination under electric drivings.

Plenary 5 (Tue 22, 09:00-10:00)

87	**Subcycle Videography of Electronic Quantum Motion**	Rupert Huber	Plenary talk

Rupert Huber (1)

(1) University of Regensburg, Germany

In lightwave electronics, optical carrier fields act as alternating voltages to accelerate electrons within less than a cycle of light. This way, crystal electrons can move without scattering, unleashing an all-coherent quantum world full of promise for future quantum technologies [1].
Subcycle dynamics, such as Bloch oscillations, quasiparticle collisions, and spin-polarized topological currents [2] manifest in high-harmonic and high-order sideband generation. Subcycle photoelectron spectroscopy can visualize the underlying dynamics with direct band-structure videography, resolving ballistic motion of Dirac currents and Floquet-Bloch band engineering [3]. By combining this idea with photoelectron momentum microscopy, we can image subcycle electron dynamics throughout the entire first Brillouin zone of essentially any quantum material [4]. Moving from momentum space to real space, lightwave-driven scanning tunnelling microscopy (STM) can videotape single molecules [5] and atomic defects [6] and observe the subcycle quantum flow of electrons [7]. By biasing the STM junction with phase-controlled single-cycle near-infrared light pulses, we combine attosecond temporal with atomic spatial resolution, for the first time [8]. Our results offer a radically new way of watching and controlling elementary quantum dynamics in condensed matter at the space-time limit.

[1] Borsch et al., Nat. Rev. Mater. 8, 668 (2023), Kira et al., Opt. & Photon. News 36, 28 (2025)
[2] Schmid et al., Nature 593, 385 (2021), Freudenstein et al., Nature 610, 290 (2022), Riepl et al., under review
[3] Ito et al., Nature 616, 696 (2023), Reimann et al., Nature 562, 396 (2018)
[4] Eggers et al., arXiv:2602.12844, under review
[5] Cocker et al., Nature 539, 263 (2016), Peller et al., Nature 585, 58 (2020)
[6] Roelcke et al., Nature Photon. 18, 595 (2024)
[7] Siday et al., Nature 629, 329 (2024)
[8] Maier et al., arXiv:2507.10206, accepted in principle

Plenary 6 (Tue 22, 14:30-15:30)

91	**Piezoelectric Thin Films Deposited from the Vapor Phase for Smart Sensors and Beyond**	Anna Maria Coclite	Plenary talk

Anna Maria Coclite (1)

(1) University of Bari

Piezoelectric microelectromechanical systems (piezoMEMS) provide a versatile platform to exploit electromechanical coupling at the microscale, enabled by the intrinsic crystalline anisotropy of piezoelectric materials. The interplay between structure and polarization allows the conversion of electrical stimuli into mechanical deformation (converse effect), as well as mechanical excitations into electrical signals (direct effect), underpinning applications in sensing and energy conversion.
In this context, piezoelectric thin films play a central role, as their structural, morphological, and interfacial properties directly determine the efficiency of electromechanical transduction. Plasma-enhanced atomic layer deposition (PEALD) offers a powerful route to engineer such properties, enabling conformal growth of ultrathin ZnO films with precise thickness control and tunable crystallinity at low temperatures. These features are particularly relevant for integration on complex and three-dimensional architectures, as well as for flexible platforms.
Here, we discuss the emerging landscape of ZnO-based piezoelectric systems, focusing on the relationship between thin film growth, nanoscale structure, and functional response. PEALD-grown ZnO films are explored in the context of wearable and electronic skin (e-skin) sensors. In addition, hybrid systems obtained via vapor phase infiltration (VPI) enable the realization of compliant three-dimensional architectures and maskless patterning, opening new opportunities for mechanically adaptive devices. Finally, direct atomic layer processing (DALP) approaches are introduced as a route to locally define piezoelectric functionality within patterned structures.
Overall, this contribution highlights how plasma-assisted approaches enable the control of structure–property relationships in ZnO thin films, bridging the gap between fundamental material properties and functional piezoelectric architectures for sensing and energy conversion.

Plenary 7 (Wed 23, 09:00-10:00)

118	**Electronic Conduction in 1D – The 0.7 and Fractions in the 1D-2D Transition**	Michael Pepper	Plenary talk

Michael Pepper (1)

(1) University College London

Confinement of a 2D electron gas to form a 1D system allows observation of conductance quantization with values of 2ne2/h where the integer n is 1,2,3,4 and the factor of 2 is spin degeneracy. This formula is based on spatial quantization and ballistic conduction. However, in 1996 a deviation from this simple behaviour occurred when a conductance plateau, or structure, was found near 0.7(2ne2/h) taking the name 0.7 structure. It is often a conductance plateau and can be between 0.8 and 0.6, the initial description of the effect was attributed to spin polarization arising from a ferromagnetic coupling, which resulted in only one spin direction being transmitted in a longer sample, with partial transmission of the other spin in a shorter sample. It is found that the conductance below the 0.7 is spin polarised. Both thermal and noise measurements indicate that the spins split with only one fully transmitted, application of a magnetic field which lifts the spin degeneracy of the plateaus also reduces the 0.7 to 0.5, ie a complete spin polarisation. It has been suggested that the spins are polarised but the polarisation axis slowly rotates in time which is consistent with the experiments.
When the confinement is weakened the 0.7 disappears, as do the first integer plateaus, and can be replaced by a new quantization with fractional values such as 1/6, ½, 1/5 and 2/5 in units of e2/h. This Non-Magnetic Fractional Quantization may be thought to have certain similarities to the Fractional Quantum Hall Effect except that there is no magnetic field, the fractions can be even as well as odd and there is no filling factor to determine the fractional value. This effect has been found in a range of semiconductors such as electrons in GaAs, InGaAs, InAs and holes in GaAs. These effects will be discussed along with possible theoretical explanations.

Plenary 8 (Wed 23, 09:00-10:00)

45	**Inverse Bicontinuous and Discontinuous Lyotropic Liquid Crystal Phases of Lipids: From Bulk Phases, to Lipid Nanoparticles**	John Seddon	Plenary talk

John Seddon (1)

(1) Imperial College London

Lyotropic liquid crystals of 1-, 2-, or 3-dimensional periodicity spontaneously assemble when lipids are mixed with aqueous solvent under various conditions of temperature, pressure and hydration. The most relevant non-lamellar phases from a biological perspective are the inverse hexagonal HII phase, and the inverse cubic phases. There are two quite distinct types of inverse cubic phase: bicontinuous ones based on underlying periodic minimal surfaces, and discontinuous ones based on simple or more complex packings of discreet inverse micelles.
In this lecture I will briefly review lipid self-assembly, interfacial curvature and phase diagrams. I will then go on to describe how the phase behaviour can be controlled, and the structure of lyotropic phases can be tuned, by various parameters such as temperature, hydrostatic pressure, or the addition of amphiphilic molecules such as fatty acids, diacylglycerols, and cholesterol. For potential medical applications, bulk lipid phases can be dispersed into lipid nanoparticles of the order of 100 – 200 nm in diameter. These are named hexosomes when formed from the HII phase, cubosomes when based on inverse bicontinuous cubic phases, and micellosomes when based on discontinuous cubic phases. It is important to consider whether the internal structure has been disrupted or modified upon converting bulk phases into lipid nanoparticles.
By incorporation of charged phospholipids, we have been able to swell inverse bicontinuous cubic phases to lattice parameters of approx. 500 Å, with water channels of approx. 220 Å diameter, po-tentially expanding the range of usefulness of such phases for applications such as drug delivery or encapsulation of enzymes [1, 2]. We have shown that cubosomes formed from these lipids can be swollen by charged lipids and also by cholesterol, and can show increased incorporation of the lec-tin PHA-L, a tetrameric protein of 120 kDa upon swelling [3].
We have previously shown that by addition of weakly-polar amphiphiles such as diacylglycerols to phospholipids, we can tune the interfacial curvature to be strongly inverse, leading to the formation of a discontinuous cubic phase of spacegroup Fd3m, with a structure based upon a complex close packing of two types of quasi-spherical inverse micelles. We investigated the effect of hydrostatic pressure on the structure and stability of this phase, and discovered a number of novel effects [4].
We have dispersed this bulk Fd3m phase into 'micellosomes' by sonication in the presence of the amphiphilic block copolymer F127, and have used x-ray diffraction to compare their structure to that of the bulk Fd3m cubic phase (A.M. Sartor et al., unpublished data). We have recently demonstrated that Fd3m micellosomes can be formed in buffer at pH 7.4 by mixtures of monoolein and oleyl alcohol, containing a small amount of an ionizable lipid. By lowering the pH to below pH 6, the zwitterionic lipid becomes cationic, triggering a phase transition within the lipid nanoparticle from an internally-confined Fd3m structure (micellosome), to a more porous inverse hexagonal HII phase (hexosome), favouring release of any encapsulated contents. We have used a combination of small-angle x-ray scattering and cryo-TEM to determine the detailed internal structure within the Fd3m micellosomes [5].
We have developed a microfluidic hydrodynamic focussing technology for the production of cubosomes and hexosomes, whose size is relatively monodisperse and can be controlled by varying the flow rate ratio between the aqueous buffer and ethanolic streams [6].
Some time ago [7] we discovered a lyotropic phase of space group P63/mmc, whose structure is based upon a 3-D hexagonal packing of quasi-spherical inverse micelles, in a hydrated mixture of dioleoyl phosphatidylcholine, dioleoyl glycerol, and cholesterol. This phase is expected to have a greater chain packing frustration than the Fd3m cubic phase, and it appears that the cholesterol is able to relieve the chain packing frustration within the hydrophobic region of this phase, allowing the P63/mmc phase to form.

[1] A.I.I. Tyler, H.M.G. Barriga, E.S. Parsons, N.L.C. McCarthy, O. Ces, R.V. Law, J.M. Seddon, and N.J. Brooks, Soft Matter 1, 3279 (2015).
[2] H.M.G. Barrriga, A.I.I. Tyler, N.L.C. McCarthy, E.S. Parsons, O. Ces, R.V. Law, J.M. Seddon, and N.J. Brooks, Soft Matter 11, 600 (2015).
[3] H.M.G. Barriga, O. Ces, R.V. Law, J.M. Seddon, and N.J. Brooks, Langmuir (2019) 35, 16521-16527.
[4] A.I.I. Tyler, G.C. Shearman, N. J. Brooks, H. Delacroix, R. V. Law, R.H. Templer, O. Ces, and J. M. Seddon, PCCP 13, 3033 (2011).
[5] Z. Xu, Zexi, J.M. Seddon, P.A. Beales, M. Rappolt, and A.I.I. Tyler, JACS (2021), 143, 40, 16556-16565.
[6] C.P. Pilkington, C. Contini, J.D. Barritt, P.A. Simpson, J.M. Seddon, and Y. Elani, Scientific Reports (2023) 13:12684.
[7] G.C. Shearman, A.I.I. Tyler, N.J. Brooks, R.H. Templer, O. Ces, R.V. Law, and J.M. Seddon, J. Am. Chem. Soc. 131, 1678 (2009).

Plenary 9 (Wed 23, 14:30-15:30)

570	**Let's Get Real - Adapting the Toolkit of Many-Body Theory to Realistic Material Simulation**	Emanuel Gull	Plenary talk

Emanuel Gull (1,2)

(1) University of Michigan
(2) University of Warsaw

Quantum many-body theories are used to describe the physics of quantum systems with many strongly interacting particles. In condensed matter physics, these theories are typically applied to effective low-energy lattice models, which are designed to capture only the essential degrees of freedom of a solid. Such models contain phenomenological parameters and are often not predictive.
This talk will summarize recent progress on solving the many-body problem ab-initio, i.e. without adjustable parameters and without the construction of effective low-energy models. We will showcase algorithmic and computational advances that have enabled high-precision calculations of solids with strong quantum effects. A path towards controlled and adaptive many-body simulations is outlined.

Plenary 10 (Thu 24, 09:00-10:00)

547	**Understanding Stellar Magnetic Activity Through Solar Physics**	Alexander Shapiro	Plenary talk

Alexander Shapiro (1)

(1) University of Graz

Magnetic activity is a fundamental property of cool stars with convective envelopes and a key driver of their variability. Our physical understanding of stellar magnetic activity is rooted in the Sun, where high-resolution observations have revealed how magnetic field modifies near-surface convection leading to the formation of different magnetic features such as dark sunspots and bright faculae. State-of-the-art magnetohydrodynamic simulations of stellar atmospheres, combined with detailed radiative transfer calculations, now allow us to model magnetic features from first principles and, crucially, to extend the solar-based framework to other stars. This extension has become particularly timely given the wealth of high-precision stellar observations produced by exoplanet missions and surveys, which have uncovered a rich variety of activity signatures caused by stellar surface magnetic features. These signatures are

both a blessing and a curse: they offer invaluable diagnostics of stellar magnetism while directly interfering with the detection and characterization of exoplanets. In this talk, I will present recent efforts to model and interpret them within a unified modeling framework connecting solar and stellar approaches.

Plenary 11 (Thu 24, 09:00-10:00)

202	**Next-Generation Particle Accelerators: Overview and Outlook**	Edda Gschwendtner	Plenary talk

Edda Gschwendtner (1)

(1) CERN

Particle accelerators have been the cornerstone of experimental high-energy physics for over a century and the quest for higher energies and luminosities continues to drive innovation in accelerator science. Following the European Strategy for Particle Physics roadmap, the community is actively preparing for the post-LHC era, with next-generation accelerator technologies under development across a broad front. This talk surveys the landscape of emerging accelerator concepts, from large-scale conventional projects to radically novel approaches. We discuss future circular and linear collider designs (e.g. FCC-ee, CLIC,...), alongside advanced technologies such as plasma wakefield acceleration and muon colliders. For each, we assess current technical readiness and the key remaining challenges on the path from proof-of-principle to a deployable machine. The aim is to provide a broad overview of this rapidly evolving field, identifying which technologies are approaching maturity and where the most significant open questions remain.

Plenary 12 (Thu 24, 14:30-15:30)

821	**tba**	Harald Reichert	Plenary talk

Harald Reichert (1)

(1) DESY, Hamburg

Plenary 13 (Fri 25, 09:00-10:00)

818	**Towards realistic pressures in X-ray photoelectron spectroscopy applied to heterogenous catalysis - and what that has tought us so far**	David Degerman	Plenary talk

David Degerman (1)

(1) Department of Physics Stockholm University AlbaNova University Center SE-106 91 Stockholm, Sweden

From simple molecular feedstocks, energy-dense and processable chemicals can be synthesized over heterogeneous catalysts. From a surface chemical physics perspective, these reactions can be modelled as a series of elementary reaction steps funneled through a potential energy landscape. A mechanistic understanding of these processes is of essence, as it enables tuning of the catalyst's activity and selectivity. To to gain this knowledge, we require techniques that (1) are surface sensitive, (2) provide high chemical specificity, and (3) are compatible with operating conditions. While X-ray photoelectron spectroscopy (XPS) has traditionally fulfilled the first two criteria, it has been largely limited to near-vacuum environments. We have developed instrumentation that helps close this “pressure gap,” enabling studies at more realistic conditions than previously possible.
This talk presents key insights enabled by these advances. By observing the adsorbate populations present under steady-state reaction conditions, we can directly compare experiments with predictive theoretical models of catalytic selectivity. This approach is particularly powerful for systems where the catalyst undergoes reaction-induced chemical changes, which are difficult to capture in silico. We demonstrate the influence of various promoters in ammonia synthesis, how different carbide species both enable - and partake in - the Fischer–Tropsch reaction, and how the state of bimetallic methanol synthesis catalysts evolves with reactant composition. Lastly, we provide an outlook for how continued development of instrumentation can increase the industrial relevance of fundamental catalysis research, and ultimately make the chemical industry both more sustainable and effective.

Semi-Plenary Talks

Semi-Plenary 1 (Mon 21, 14:30-15:00)

ID	Title	Speaker	Type
33	**Spin-Directed Chiral Symmetry Breaking**	Yves Geerts	Semi-Plenary talk

Yves Geerts (1)

(1) Free University of Brussels (ULB) & International Solvay Institutes, Belgium

Louis Pasteur and Pierre Curie dreamed of directing chiral symmetry breaking using external magnetic and electric fields. [Chem. Rev. 1998, 98, 2391] Their attempts failed due to time-inversion symmetry, theoretically explained by Laurence Barron. [JACS 1986, 108, 5539] Dissipative non-equilibrium conditions break this symmetry and allow the separation of enantiomers under the influence of false chirality, as recently demonstrated by Ron Naaman and Francesco Tassinari. [Chem. Sci. 2019, 10, 5246. Cryst. Growth Des. [2021, 21, 2925] With my team, we have undertaken a research project aimed at going further by directing deracemization towards R or S enantiomers using chirality-induced spin selectivity (CISS). [Acc. Chem. Res.] [2020, 53, 2659] I will report on our latest results and the prospects for realizing Pasteur and Curie's long-held dream.

Semi-Plenary 2 (Mon 21, 15:00-15:30)

623	**Peculiar Phenomena of 2D World from Surface Science Perspective**	Pawel Kowalczyk	Semi-Plenary talk

Rafał Dunal (1) Paweł Dąbrowski (1) Pawel Kowalczyk (1) Witold Kozłowski (1) Paweł Krukowski (1) Iaroslav Lutsyk (1) Aleksandra Nadolska (1) Michał Piskorski (1) Przemysław Przybysz (1) Łukasz Radecki (1) Maciej Rogala (1) Wojciech Ryś (1) Jagoda Seroka (1) Karol Szałowski (1) Klaudia Toczek (1)

(1) University of Lodz, Poland

Two-dimensional (2D) materials provide a unique playground in which reduced dimensionality, surface effects, and interfacial interactions give rise to electronic and structural phenomena absent in bulk systems. Among others we focused on 2D elemental systems based on 15th group α-antimonene, α-bismuthene. Following the synthesis of these systems, we have systematically explored their physical properties, uncovering a range of intriguing phenomena. These include unpinned Dirac states [1], Dirac points enforced by nonsymmorphic symmetries [2], and signatures of topologically protected edge states [3]. More recently, we reported directional structural superlubricity and indications of Lévy-flight-like dynamics in the spontaneous diffusion of Bi nanostructures on graphite [4]. However, these materials are inherently prone to environmental instability, which motivated us to undertake a broader investigation of oxidation processes at the nanoscale, extending our studies to a wider class of 2D systems and exploring strategies for their stabilization.
A key challenge in the study and application of 2D materials is their susceptibility to oxidation, which limits experimental reproducibility and device stability. In this context, we have systematically investigated the oxidation behavior of TMDs, revealing a pronounced thickness dependence near the monolayer limit. Ultrathin layers exhibit oxidation pathways distinct from their bulk counterparts, leading to the formation of structurally and electronically distinct oxide phases.
One strategy to mitigate degradation is the use of protective capping layers. We have explored several such approaches, with particular emphasis on graphene. Beyond its protective role, graphene enables the formation of heterostructures with TMDs, providing a platform to engineer its electronic properties, including attempts to induce a band gap and to investigate twist-dependent phenomena.
At the same time, rather than treating oxidation solely as a detrimental effect, we exploit oxide formation as a route toward functional materials. In particular, we investigated the controlled growth of ultrathin MoO_3 layers on graphite [5, 6], demonstrating a substantial increase in its work function (WF), which is essential for applications such as optoelectronic devices. Moreover, MoO_3-based systems provide a versatile platform for functional phenomena, including resistive switching, which will also be discussed.

[1] Q. Lu et al., Nat. Comm. 13 (2022) 4603
[2] P.J. Kowalczyk et al., ACS Nano 14 (2020) 1888
[3] S. Salehitaleghani et al., 2D Mat. 10 (2022) 15020
[4] M. Le Ster et al., Small 21 (2025) 2408349
[5] D. Kowalczyk et al., 2D Mat. 8 (2021) 25005
[6] D. Kowalczyk et al., ACS Appl. Mat. Int. 14 (2022) 44506

This work was supported by National Science Centre, Poland under projects: 2019/35/B/ST5/03956, 2020/38/E/ST3/00293 and 2024/55/B/ST11/01717.

Semi-Plenary 3 (Wed 23, 14:30-15:00)

805	**Magnetically controlled optical effects in Eu-based conductors**	Ana Akrap	Semi-Plenary talk

Ana Akrap (1)

(1) Department of Physics, University of Zagreb, Croatia

Europium is a fascinating element. In its 2+ valence state, it has a large spin of 7/2. In this talk, we will delve into what we learned about $EuCd_2X_2$ (where X= As, P and Sb) from infrared spectroscopy and magneto-optical experiments. Although we had initially hoped to find evidence of a magnetic Weyl semimetal, instead we found multiple experimental confirmations of a sizeable band gap, just shy of 1 eV.

Most interesting, however, is our finding that the band gap is remarkably sensitive to a small external magnetic field. $EuCd_2X_2$ starts off as an antiferromagnet in zero external field, but becomes fully spin polarized already below 2 T. A large exchange coupling between the f-states and the conduction and valence bands shrinks the band gap by 20% under only 2 T in $EuCd_2As_2$. The splitting of the bands reaches about 240 meV.

We will discuss how this strong influence of magnetism on conducting states leads to several remarkably strong and potentially useful optical effects in $EuCd_2X_2$.

Semi-Plenary 4 (Wed 23, 15:00-15:30)

795	**3D Printed Micro-Optics: Fundamentals and First Hallmark Applications**	Harald Giessen	Semi-Plenary talk

Harald Giessen (1)

(1) University of Stuttgart, Germany

Semi-Plenary 5 (Thu 24, 14:30-15:00)

648	**Chiral Phononics: A New Approach to Angular Momentum in Solids**	Dominik Juraschek	Semi-Plenary talk

Dominik Juraschek (1)

(1) Eindhoven University of Technology, The Netherlands

Chiral phononics is an emerging field that utilizes the angular momentum of circularly polarized lattice vibrations to manipulate the properties of quantum materials. This has led to intriguing discoveries of emerging phenomena, including phononic analogues of spintronic and orbitronic effects, as well as the generation of atomistic tesla-scale magnetic fields that promise unprecedented control of magnetic order. In this talk, I will provide an introduction to the field and then present recent predictions of novel physical mechanisms from my group. Specifically, I will present a theory for the phonon angular momentum Hall effect that induces a transverse angular-momentum current and accumulation similar to the spin and orbital Hall effects for electrons. I will further show how chiral-phonon scattering leads to a rotational analogue of the Umklapp process in solids, demonstrating the conservation of crystal angular momentum.

Semi-Plenary 6 (Thu 24, 15:00-15:30)

192	**Fisher Information in Electromagnetism**	Stefan Rotter	Semi-Plenary talk

Stefan Rotter (1)

(1) TU Wien, Austria

In my talk, I will discuss recent progress in applying the concept of classical and quantum Fisher information to the problem of estimating system parameters in electromagnetic scattering and nano-photonics. Specifically, I will demonstrate how Fisher Information can be maximised through wavefront shaping and quantum state engineering [1,2]. Quite remarkably, the density and flux of Fisher information satisfy a fundamental continuity equation – in analogy to the Poynting theorem for the density and flux of energy in a radiation field [3]. This viewpoint allows us to identify Fisher information as a physical quantity that propagates through space and that can resonate, diffract, and interfere [4]. Finally, I will also discuss how such concepts can be generalised to the flow of Fisher Information through Artificial Neural Networks [5].

[1] Maximum information states for coherent scattering measurements, D. Bouchet, S. Rotter, and A. P. Mosk, Nature Physics 17, 564 (2021).
[2] How to find optimal quantum states for optical micromanipulation and metrology in complex scattering problems, L. M. Rachbauer, D. Bouchet, U. Leonhardt, and S. Rotter, J. Opt. Soc. Am. B 41, 2122 (2024).
[3] Continuity equation for the flow of Fisher information in wave scattering, J. Hüpfl, F. Russo, L. M. Rachbauer, D. Bouchet, J. Lu, U. Kuhl, and S. Rotter, Nature Physics 20, 1294 (2024).
[4] Controlling the flow of information in optical metrology, M. Weimar, H. Zhou, L. Neubacher, T. A. Grant, J. Hüpfl, K. F. MacDonald, S. Rotter, and N. I. Zheludev, arXiv:2508.13640
[5] Fisher information flow in artificial neural networks, M. Weimar, L. M. Rachbauer, I. Starshynov, D. Faccio, L. Adilova, D. Bouchet, and S. Rotter, Phys. Rev. X 15, 031072 (2025).

AWS – Award Winner Session and ERC

AWS – Session 1 (Wed 23, 10:30-12:30)			
ID	Title	Speaker	Type
	Roman Ulrich Sexl Prize	tba	Invited talk (10:30-11:00)
	Fritz Kohlrausch Prize	tba	Invited talk (11:00-11:30)
	Auwärter Prize	tba	Invited talk (11:30-12:00)
815	**European Research Council (ERC) - Funding Opportunities and Guide for Prospective Applicants**	Odeta Limaj	Invited talk (12:00-12:30)

Odeta Limaj (1)

(1) ERC, Brussels

The European Research Council (ERC) is a research funding body aimed at supporting frontier research in all fields of science. The ERC received a budget of over 16 billion Euro under the European Union research programme Horizon Europe. Currently, it has funded more than 14 000 top researchers in the domains of life sciences, physical sciences and engineering and social sciences and humanities.
In this talk, we will give an overview of the ERC funding schemes (Starting, Consolidator, Advances, Synergy and ERC PLUS Grants), describe the evaluation process and provide a step-by-step guide and tips for prospective applicants.
More information can be found at: https://erc.europa.eu/

AKCP - Equal Opportunities in Physics

AKCP – Session 1 (Mon 21, 16:00-18:00, Chair: Ille Gebeshuber)			
ID	Title	Speaker	Type
	Berta Karlik Poster Award Session		

AKCP – Session 2 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
817	**Navigating the Physics Landscape: My Personal Path to Empowering Equality**	Manuela Stadlober-Temmer	Invited talk (16:00-16:30)

Manuela Stadlober-Temmer (1)

(1) Institute for Physics, University of Graz

Academic success is often measured by publications, grants, and awards. Yet, the journey behind these achievements is rarely discussed. Academic careers often do NOT follow a straight line and comparison with others can be easily misleading and frustrating. As community we should rather focus on growth than on competition, because what matters in science is persistence and curiosity. But, this is usually not in line with performance records asked by institutions to get financial support for science (and a fixed position).
The narrative about my own career should therefore be only a start for raising discussions about empowerment in physics such as () robust mentorship programs that provide guidance and visibility, () targeted initiatives for early-career support to bridge the "leaky pipeline," and (*) institutional change through policy reform that embeds equity into the core of research organizations.

151	**GENERA Network: 10 years Exchange and Activities on Gender Equality in Physics in Europe**	Thomas Berghoefer	Invited talk (16:30-17:00)

Thomas Berghöfer (1)

(1) Deutsches Elektronen Synchrotron (DESY)

GENERA Network is the collaboration in advancing gender equity and further promoting diversity and inclusion throughout physics research communities in Europe. This network originated from the GENERA project, which was funded by the European Commission from 2015-2018. In this project 11 physics research institutions and two support organizations received funding to developed and implemented Gender Equality Plans (GEPs) together. The basic idea for a continuous networking beyond this project was, first, to monitor the long-term impact of the GEPs. Second, to organize a continuous exchange of good-practice and, third, to perform common activities.
This contribution presents the motivation, goals, and activities of the GENERA Network and outlines opportunities for participation. In particular, the presentation will focus on the ERASMUS+ project GENERA-COPA, which was launched last year and addresses the question of the existence of a gender or diversity perspective as well as developing innovative approaches in education and mentoring in physics and other math-intensive STEM fields.

254	**Physics Needs Everyone: The Atom*innen Platform as a Tool for Equity and Change**	Karoline Irschara	Invited talk (17:00-17:30)

Karoline Irschara (1)

(1) Institut für Quantenoptik und Quanteninformation, Österreichische Akademie der Wissenschaften, Innsbruck

In Europe, the average representation of women in physics remains strikingly low – a challenge that physics shares with other STEM subjects. According to Eurostat, the proportion of female bachelor's degree students in physics has barely changed since 2015, remaining at around 30%. The gender imbalance becomes particularly evident at senior levels: in Austria, for example, women hold only around 13% of physics professorships, similar to the situation in Germany where the figure is around 12%.
While the need for greater inclusion is widely acknowledged, translating this awareness into concrete action remains a major challenge. In this talk, I will examine gender representation in physics in Austria and across Europe, and present atom*innen, an interactive platform designed to connect and support women and gender minorities in quantum physics. I will outline the motivation, goals, and activities behind the platform, and discuss how it can serve as an open space where members can connect, collaborate, and drive change together.

490	**Progress towards Th-229 Nuclear Clock Development**	Ira Morawetz	Invited talk (17:30-18:00)

Ira Morawetz (1)

(1) Vienna Center for Quantum Science and Technology, Atominstitut, TU Wien

Thorium-229 has a low-energy nuclear transition that has been excited in thorium-doped crystals with laser light. This opens the perspective towards a highly stable and robust solid-state optical nuclear clock. We report recent progress in exciting the nucleus with a continuous-wave laser source and that the resonance signal can be detected in absorption rather than in fluorescence. This eliminates the slow nuclear fluorescence decay from the detection process and offers a considerable advantage for clock operation through fast signal acquisition.

AKCP – Poster session (PS1 Mon21-Tue22)			
ID	Title	Presenter	Type
46 **P031**	**TUgether ohne Barrieren: A Physics-Informed Approach to Inclusive Academic Environments with a Focus on Twiceexceptional Individuals**	Ille C. Gebeshuber	Poster

Ille C. Gebeshuber (1) Lisa Marx (1) Pia M. Graves (1) Marion Hersh (2)

(1) TU Wien
(2) Glasgow University

Ensuring equal opportunities in physics requires not only formal access, but also a deep understanding of systemic barriers that affect participation, performance, and creativity. The project TUgether ohne Barrieren, led at TU Wien in collaboration with the University of Glasgow, addresses these challenges through an interdisciplinary, evidence-based framework grounded in analytical thinking familiar to the physical sciences.
The project applies quantitative and qualitative methodologies—anonymous large-scale surveys and structured interviews—to identify barriers in infrastructure, teaching, and institutional processes. From a physics perspective, the university system can be viewed as a complex system with constraints, boundary conditions, and non-linear responses to interventions. Within this system, particular attention is given to twiceexceptional (2e) individuals: persons with high cognitive or creative abilities who simultaneously experience disabilities or neurodivergent conditions (e.g., autism, ADHD, dyslexia). These individuals often exhibit exceptional pattern recognition, abstraction capabilities, or problem-solving skills—traits highly valuable in physics —yet face disproportionate structural obstacles.
By combining empirical data analysis with international benchmarking and best-practice transfer, the project aims to derive optimized intervention strategies analogous to constraint minimization in physical systems. The expected outcome is a set of scalable, evidence-based measures that enhance accessibility while simultaneously fostering innovation, diversity of thought, and scientific excellence.
This contribution highlights how concepts familiar to physicists—such as system optimization, hidden variables, and emergent behaviour—can inform the design of inclusive academic environments, ultimately improving conditions not only for 2e individuals but for the entire scientific community.

AMP - Atoms, Molecules, Quantum Optics and Plasmas

AMP – Session 1 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
348	**Subcycle Electron-Electron Correlation Effects on High-Harmonic Generation**	Katharina Buczolich	Contributed talk (16:00-16:15)

Katharina Buczolich (1) Takeshi Sato (2) Kenichi Ishikawa (2) Fabian Lackner (1) Joachim Burgdörfer (1) Iva Brezinova (1)

(1) TU Wien
(2) The University of Tokyo

High-harmonic generation (HHG) is one of the fundamental processes at the heart of attosecond physics. Traditionally viewed as an effective single-particle effect, recent advances have focused on contributions to the harmonic spectrum beyond this single-particle picture [1, 2], as well as on probing electron correlations through HHG in atoms, molecules, and solids [3, 4]. In this work, we quantify the influence of time-dependent electron-electron correlations on HHG using correlation measures from quantum information theory. By explicitly solving the time-dependent Schrödinger equation with the multi-configurational time-dependent Hartee-Fock method [5], we obtain fully correlated results for several multi-electron atoms. When comparing different atomic species, i.e. noble gas atoms (He, Ne) with alkaline-earth atoms (Be, Mg) we find the subcycle variation of correlation parameters to differ markedly for noble gases and alkaline-earth atoms. We provide an intuitive explanation of these surprising effects based on the dynamics of natural orbitals and discuss the effect of this ultrafast correlation dynamics on the HHG spectrum [6].

[1] A. D. Shiner et al., Nature Phys 7, 464–467 (2011).
[2] A. De Las Heras et al., Phys. Rev. Res. 2, 033047 (2020).
[3] D. R. Baykusheva et al., Phys. Rev. X 12, 011013 (2022).
[4] R. E. F. Silva et al., Nat. Photon. 12, 266 (2018).
[5] T. Sato et al., Phys. Rev. A 94, 023405 (2016).
[6] K. Buczolich et al., Phys. Rev. Res. 7, 043322 (2025).

624	**Input-Output Pulse Description of the SUPER Excitation Scheme**	Johannes Kerber	Contributed talk (16:15-16:30)

Johannes Kerber (1) Christoph Hotter (2) Helmut Ritsch (1) Klaus Mølmer (3)

(1) Universität Innsbruck
(2) Massachusetts Institute of Technology
(3) University of Copenhagen

We formulate the two-color SUPER excitation scheme for a two-level emitter within the input-output theory for quantum pulses. This provides a mode-resolved quantum description of the experimental case of two coherent traveling pulses and allows direct comparison with previous cavity-based analyses. We show that the traveling-pulse realization retains the same multiphoton character as the cavity SUPER mechanism, visible as a net photon-number change of -2 in one mode and +1 in the other. At the same time, the pulse description is not equivalent to a two-mode cavity model: a minimum pulse photon number is required to achieve high-fidelity inversion. The system also serves as a useful testbed to showcase and compare several complementary methods to solve the dynamics. To treat the large coherent-state occupations relevant for SUPER, we combine the input-output formalism with a cumulant expansion approach. With an interaction-picture formulation the few exchanged photons that govern the nontrivial dynamics enable direct full-quantum calculations in truncated Hilbert spaces, including treatments in a displacement frame and for initial Fock-state pulses.

130	**Vibrationally Induced Resonances in Few-Emitter Lasing**	Christian Schäfer	Contributed talk (16:30-16:45)

Kai Müller (1) Kimmo Luoma (2) Christian Schäfer (3)

(1) Technische Universität Dresden
(2) University of Turku
(3) TU Wien

In its extreme, nanolasers might be comprised of only a few molecules confined in plasmonic nanoresonators. Few-emitter lasers promise low energy requirements and fast responses in a footprint that can be inserted into any device or biological tissue. Utilizing the recently developed stacked hierarchy approach [arXiv:2405.05093], informed from first principles, we demonstrate the impact of vibrational structure on lasing, using the example of few-molecule lasing in plasmonic cavities. Explicitly accounting for the entire vibrational manifold unveils resonances in the laser intensity that depend on the Stokes shift, drive strength, and the number of emitters [arXiv:2604.00798]. Our work identifies limits of the omnipresent "incoherent drive"-approximation and paves the way for the understanding of nanolasers at the molecular scale.

619	**Efficient Variational Dynamics of Open Quantum Bosonic Systems via Automatic Differentiation**	Francesco Carnazza	Contributed talk (16:45-17:00)

Francesco Carnazza (1) Cristiano Ciuti (1) Luca Giacomelli (1) Jacopo Tosca (1)

(1) Université Paris Cité

We introduce a scalable variational method for simulating the dynamics of interacting open quantum bosonic systems deep in the quantum regime. The method is based on a multi-dimensional Wigner phase-space representation and employs a Variational Multi-Gaussian (VMG) ansatz, whose accuracy is systematically controlled by the number of Gaussian components. The variational equations of motion are derived from the Dirac-Frenkel principle and evaluated efficiently by combining the analytical structure of Gaussian functions with automatic differentiation. As a key application, we study a driven-dissipative two-dimensional Bose-Hubbard lattice with two-boson coherent driving and two-body losses. Using our dynamical approach, we compute the finite-size scaling of the Liouvillian spectral gap - extracted from the relaxation dynamics - which vanishes in the thermodynamic limit. Our results reveal critical slowing down with dynamical exponents of the 2D quantum Ising universality class, demonstrating the power of our method to capture complex quantum dynamics in large open systems.

690	**Free Expansion of a Charged Nanoparticle via Electrostatic Compensation**	David Steiner	Contributed talk (17:00-17:15)

David Steiner (1) Yaakov Y. Fein (1) Gregor Meier (1) Stefan Lindner (1) Paul Juschitz (1) Mario A. Ciampini (1) Markus Aspelmeyer (1) Nikolai Kiesel (1)

(1) Universität Wien

Coherent expansion of a quantum wavepacket is a necessary fundamental step in many experimental protocols to prepare, manipulate, and read out non-classical states, especially for levitated dielectric nanoparticles where the ground state extent is on the order of 10 pm. Free evolution is potentially the most straightforward technique to achieve this state expansion. While it is both a simple and effective expansion scheme, it does require compensation of static forces to avoid mean displacement of the wavepacket during the free evolution.
Using an optical trap-release-recapture sequence involving a charged nanoparticle we developed methods to measure and counteract static forces. Compensating gravity and stray electric fields, in three dimensions, we demonstrate free evolution for 1 ms with subsequent recapture. Coupled with a short harmonic pulse in between two free expansions, we have performed recompression and time-of-flight protocols, speaking for the coherence of our approach as well as its usefulness to further generate squeezed mechanical states.

117	**Towards Trapping and Cooling Techniques for Levitated Dielectric and Biological Nanoparticles**	Stefan Schrems	Contributed talk (17:15-17:30)

Markus Arndt (1) Florian Fechtel (1) Lorentz Hummer (1) Stefan Schrems (1) Stephan Troyer (1) Jean Paul Louys Sanso () Tracy Eleanor Northub (2) Roland Wester (3) Samuel White (3)

(1) Universität Wien, Fakultät für Physik
(2) Universität Innsbruck, Department of Experimental Physics
(3) Universität Innsbruck, Department of Ion Physics and Applied Physics

Matter-wave interferometry has recently been demonstrated for particles as massive as metal nanoclusters exceeding 170kDa. Extending this frontier into the 10-50MDa regime of dielectric or biological nanoparticles is now a compelling open challenge in quantum physics, aiming for the preparation of Schrödinger cat states at unprecedented mass scales. Future interferometry experiments in this regime require slow, mass-selected, cold nanoparticles. Recent breakthroughs in levitated optomechanics achieved cooling of trapped nanoparticles with 0.1-5GDa mass to their motional or librational quantum ground state using coherent scattering or feedback cooling. For particles with a radius of r = 10-30nm, conventional Rayleigh detection and feedback is challenging as it scales with polarizability and mass like α^2 ($\alpha \propto m$). Additionally, laser-induced heating of biological particles must also be minimized. We therefore study electric feedback cooling in an electrodynamical ion trap with interferometric readout (homodyne /heterodyne), which scales only linearly in polarizability and mass. We characterize the trapping of dielectric and biological nanoparticles in a Paul trap and their detection via a 532nm CW laser.

207	**Measurements of Positronium Compound Binding Energies**	Ross Edward Sheldon	Contributed talk (17:30-17:45)

Daniel James Murtagh (1) Ross Edward Sheldon (2) Alina Weiser (2)

(1) Imperial College London
(2) Marietta Blau Institute, Austrian Academy of Sciences

Positronium (Ps), the short-lived bound state of an electron and its antimatter counterpart the positron, can form a variety of exotic molecular systems. Although theoretical studies predict the existence of more than thirty Ps compounds [1], experimental observation remains limited to the simplest systems, positronium hydride (PsH) [2] and deuteride (PsD) [3]. Ps compounds are relevant in multiple fields, including many-body quantum calculations [1], materials studies [3], and antihydrogen ion formation [4], but the lack of experimental results means calculations are unvalidated. We report a renewed experimental effort to search for and characterise these molecules, such as PsH, PsO and PsF, by measuring their binding energy with a precision of approximately 50 meV.
To this end, we have constructed a dedicated positron beamline based on a ^{22}Na source, a Surko-type buffer-gas positron trap, and a 1 amu resolution time-of-flight mass spectrometer. The trap produces positron bunches characterised by a narrow energy spread of 59 ± 1 meV. Ps compounds are formed via collisions between the positron beam and an effusive molecular gas-jet target $e^+ + AB \rightarrow A^+ + PsB$, employing a methodology analogous to that used in Ref. [2]. The ion produced in the collision is identified in a time-of-flight mass spectrometer using a microchannel plate detector (MCP), its appearance below the threshold for Ps production indicating if the Ps compound is made.
We present the first measurements of this experiment and compare them to the available theoretical models.

[1] X. Cheng et al., Phys. Rev. A 85, 012503 (2012).
[2] D. M. Schrader et al., Phys. Rev. Lett. 69, 57 (1992).
[3] M. A. Monge et al, J. Radioanalytical and Nuclear Chem. 211, 23-29 (1996).
[4] J. Taylor et al., Phys. Rev. A 109, 052816 (2025).

131	**Prediction of Molecular Single-Photon Emitters: A Materials-Modeling Approach**	Christian Schäfer	Contributed talk (17:45-18:00)

Erik Öhman (1) Daqing Wang (2) Matthias Geilhufe (1) Christian Schäfer (3)

(1) Chalmers University of Technology
(2) University of Bonn
(3) TU Wien

Interfacing light with quantum systems is an integral part of quantum technology, with the most essential building block being single-photon emitters. Although various platforms exist, each with its individual strengths, molecular emitters boast a unique advantage: the flexibility to tailor their design to fit the requirements of a specific task. However, the characteristics of the vast space of possible molecular configurations are challenging to understand and explore. Here, we present a theoretical and computational framework to initiate exploration of this vast potential by integrating database analysis with microscopic predictions. Using a model system of dibenzoterrylene in an anthracene host as benchmark, our approach identifies promising new candidates, among them a chiral molecular emitter. [https://doi.org/10.1103/11bh-ywcc]

AMP – Poster session (PS1 Mon21-Tue22)			
ID	Title	Presenter	Type
101 **P032**	**Bichromatic Laser Deceleration and Cooling of Hot Positronium**	Barna Mendei	Poster

Barna Mendei (1) Helmut Ritsch (1)

(1) Universität Innsbruck

We study laser cooling and trapping of hot para-positronium bunches as produced by a Surko trap. While laser cooling via radiation pressure is a very well established technique to slow and cool down neutral atoms below mK, the fast ground state annihilation and high recoil shift poses challenging extra limitations on the required laser powers and frequencies. Some earlier work suggests viable prospects for obtaining a cold sufficiently dense ensemble nevertheless. Our theoretical study sets out to explore new ways for these exotic atoms beyond simple Doppler-cooling on the 1^3S-2^3P transition by including an extended upper state manifold and extra transverse lasers on the 2^3P-3^3D transition. The specific objective of this study was to examine the effect of this additional excitation on the quality of positronium atoms' cooling process. This research employs semi-classical approaches of simulating light-matter interactions. We successfully found experimentally reasonable values for the lasers' parameters, whose proper application can lead to an effective slowing of positronium. With the presented scheme we were able to achieve an acceptable and fast slowing effect while the majority of atoms were not annihilated. Future extension to collective cooling and trapping in cavities or hollow core fibres could be the basis of new discoveries in the investigation of cold Ps systems even pointing towards superradiant lasing and Bose-Einstein-condensates.

384 **P033**	**Ultrafast Optical Field Sampling in Ambient Air**	Jakob Bancalari	Poster

Jakob Bancalari (1) Keyhan Golyari (1) David Loibner (1) Marcus Ossiander (1) Martin Schultze (1)

(1) Graz University of Technology

We present an interferometric field-sampling approach for characterizing few-cycle laser pulses, using photoionization of ambient air as the detection medium. Our method uses two replicas of the laser pulse to be sampled: one initiates sub-cycle ionization in air, while the delayed replica accelerates the released electrons and encodes the waveform in the resulting transient plasma current. By recording the current as a function of the interferometer delay, we retrieve the temporal structure of the near-infrared few-cycle field directly under ambient conditions. In addition to the self-referenced geometry, we characterize the few-cycle pulse itself, rather than a longer-wavelength field sampled with a separate few-cycle gate. The method thus combines self-referenced operation, broadband sensitivity, and experimental simplicity, providing a compact tool for direct waveform diagnostics in strong-field experiments.

637 **P034**	**Low Energy Crossed Beam Scattering of Cationic Noble Gases on Furan**	Christian Sprenger	Poster

Christian Sprenger (1) Viviane Schmidt (1) Roland Wester (1) Fabio Zappa (1)

(1) Universität Innsbruck, Department of Ion Physics and Applied Physics

Furan is a deceptively simple molecule. But its simple shape, a five membered ring with a single oxygen atom and four carbon atoms, each of the latter with a hydrogen atom bound to it, hides its vast potential. Furan (and its derivates), obtained from biomass, are being regarded as an alternative resource for chemical industry, replacing fossile alternatives [1]. Furthermore furan rings look promising to improve the power conversion efficiency of organic solar cells [2] and applications of furan ring structures in medical drugs have been studied [3].
Here we study collision induced dissociation of Furan. We have performed low energy scattering experiments of the neutral furan molecule with He^+ and Ne^+. These experiments were performed at low energies, below 5 eV, within a velocity map imaging spectrometer, analysing the collisions at a molecular level. This has proven to be a powerful technique for the analysis of ion-molecule reactions to gain deep insights into their mechanisms [4].
Here we have measured the branching ratios into several product ions. For each of those we have obtained the fragment velocity distribution. The results of these experiments will be presented.

[1] R. Bielski, G. Grynkiewicz, Green Chem., (2021) 23, 7458
[2] B. Zheng, L. Huo, Small Methods, 5, 2100493
[3] R. Banerjee, K. HKS, M. Banerjee, Int. J. Rev. Life. Sci, (2012) 2, 1, 7-16
[4] E. Carrascosa, J. Meyer, R. Wester, Chem. Soc. Rev., (2017) 46, 7498-7516

436 **P035**	**All-Optical Hyperfine Qudit Gates in Trapped Neutral Atoms**	Johannes Krondorfer	Poster

Johannes Krondorfer (1) Matthias Diez (1) Andreas Hauser (1)

(1) Graz University of Technology

Neutral atoms have emerged as a leading platform for quantum information processing. In particular, alkaline-earth and alkaline-earth-like atoms combine long coherence times, well-characterized hyperfine structure, and precise controllability via external fields. While most current implementations focus on qubits, where two internal states are selected to define an effective two-level system, the rich internal level structure of these atoms also naturally supports multi-level quantum systems. In contrast to two-level systems, these 'qudits' increase the information density per computational unit and thereby reduce circuit complexity. They allow for more efficient quantum simulations and offer new possibilities for logical encoding and error-resilient quantum information processing.
In this work, we present a fully optical approach to universal qudit control in trapped neutral atoms at moderate magnetic fields, focusing on the 1S0 → 3P1 transition in 173Yb. We show that universal single-qudit control can be achieved through single-beam Raman transitions between neighboring hyperfine states, together with state-selective phase gates. Our analysis identifies a magic polarization angle of the laser field at which the Raman couplings become state selective, suppress off-resonant mixing, and enable gate rates exceeding 100 kHz.
The same framework is compatible with non-destructive read-out via bright-state cycling transitions on the stretched states, and with two-qudit gates based on the Rydberg blockade mechanism. Taken together, these results establish 173Yb as a promising platform for fast, selective, and scalable control of nuclear-spin qudits, with clear prospects for multilevel quantum computing and quantum simulation.

COND - Condensed Matter

COND – Session 1 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
242	**Excess quasiparticles and their dynamics in the presence of subgap states**	Gianluigi Catelani	Contributed talk (16:00-16:15)

Paul Fischer (1) Gianluigi Catelani (1)

(1) Juelich Research Center and Technology Innovation Institute

Material inhomogeneities in a superconductor generically lead to broadening of the density of states and to subgap states. The latter are associated with spatial fluctuations of the gap in which quasiparticles can be trapped. Recombination between such localized quasiparticles is hindered by their spatial separation and hence their density could be higher than expectations based on the recombination between mobile quasiparticles. We show here that the recombination between localized and mobile excitations can be efficient at limiting the quasiparticle density. We comment on the significance of our findings for devices such as superconducting resonators and qubits.We find that for typical aluminum devices, the subgap states do not significantly influence the quasiparticle density.

372	**Unveiling Topological Surface States through Planar Hall Signatures in exfoliated $ZrTe_5$ flakes**	Sophia Hollweger	Contributed talk (16:15-16:30)

Rajdeep Adhikari (1) Sophia Hollweger (1) Alberta Bonanni (1) Bogdan Faina (1)

(1) Johannes Kepler Universität Linz

We report on the electronic and topological properties of $ZrTe_5$ flakes synthesized via chemical vapor transport (CVT). Mechanically exfoliated flakes with nominal thicknesses ~100 nm are transferred onto pre-fabricated Pt contacts with 1-3-3-1 Hall bar geometries on SiO_2/Si sugbstrates. Using ac phase-locked low-T/high-$\mu_0 H$ magnetotransport measurements, a distinct longitudinal resistance peak at 150 K is observed, signaling a Lifshitz transition and a subsequent crossover from hole- to electron-dominated charge carrier transport. Analysis of Shubnikov-de Haas (SdH) oscillations and observation of an anomalous Hall effect yields a non-trivial Berry phase ($\phi = \pi$), indicating the presence of topological surface states. Angle-resolved magnetotransport measurements reveal the emergence of a pronounced planar Hall effect around the transition temperature. These results characterize $ZrTe_5$ as a potential topological quantum material with applications in hybrid quantum devices such as topological Josephson junctions.

486	**Superconducting Properties of Bi-2212 Films with Thickness Below 50 nm**	Bernd Aichner	Contributed talk (16:30-16:45)

Bernd Aichner (1) Sandra Keppert (1) Johannes D. Pedarnig (2) Wolfgang Lang (1)

(1) University of Vienna, Faculty of Physics
(2) Johannes Kepler University Linz, Institute of Applied Physics

Growing thin films of the high-critical-temperature superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) is essential for fabricating nanostructures in this material using a helium ion microscope (HIM). At the beam energy of 30 keV available in the HIM, helium ions only have limited penetration depth, and their path broadens with increasing film thickness. Consequently, the film thickness is limited to just a few unit cells, but performance of such thin films is limited by the interface with the substrate at one side and with air on the other.
The films under investigation were grown by pulsed laser deposition at JKU Linz [1], patterned into stripes suitable for electronic transport measurements by optical lithography and wet-chemical etching, and post-annealed to compensate for oxygen losses that occurred during the structuring process.
From electronic transport measurements, we can derive important superconducting metrics such as the critical temperature, and the critical current at different temperatures and magnetic fields, which proved to be exceptionally high for films of this thickness [2]. Due to the high anisotropy of Bi-2212, it is essential to perform measurements with different directions of the magnetic field relative to the film surface. From these data, we derived fundamental parameters such as the in-plane and out-of-plane coherence lengths, the London penetration depth, the anisotropy factor and the Ginzburg Landau parameter. Hall effect measurements further reveal the temperature dependence of the carrier mobility, and the Hall coefficient exhibits two sign reversals – an observation that remains to be fully explained.
This work can help to better understand how to optimize electrical properties in ultrathin Bi-2212 thin films, which can potentially be nanopatterned into interesting device geometries by helium ion microscopy.

[1] S. Keppert, B. Aichner, R. Adhikari, B. Faina, W. Lang, J. D. Pedarnig: Phase Purity and Surface Morphology of High-J Superconducting BiSrCaCuO Thin Films, Appl. Surf. Sci. 636, 157822 (2023)
[2] B. Aichner, S. Keppert, J. D. Pedarnig, W. Lang: Enhanced superconducting properties of BiSrCaCuO films with sub-50-nm thickness, Sci. Rep. 15, 11855 (2025)

703	**Entropy mapping under uniaxial pressure utilizing the elastocaloric effect**	Zhenhai Hu	Contributed talk (16:45-17:00)

Zhenhai Hu (1) Andreas Rost (2) You-Sheng Li (3) Aleksei Vladimirovich Frolov (1) Naoki Kikugawa (4) Manuel Brando (1) Hilary Noad (1) Michael Nicklas (1) Andrew Mackenzie (1)

(1) Max Planck Institute for Chemical Physics of Solids
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Sr_2RuO_4 is an unconventional superconductor whose superconductivity is unusually sensitive to the underlying electronic structure and lattice symmetry. In particular, uniaxial stress provides a direct route to tuning the physics of Sr_2RuO_4: stress applied along the $\langle 100 \rangle$ direction lowers the tetragonal symmetry, modifies the Fermi surface, and drives the system toward a Van Hove singularity, where a strong enhancement of the superconducting transition temperature is observed.
As a strain-sensitive thermodynamic probe, the elastocaloric effect measures the temperature response to an oscillating strain and provides access to entropy derivatives with respect to strain. Li et al. reported a detailed implementation of this technique in Sr_2RuO_4 (Nature 607, 276–280, 2022), including the first elastocaloric mapping of a strain-tuned superconducting transition. Our analysis shows that the quasi-adiabatic regime used in Li et al. is difficult to

maintain across the experimentally relevant phase diagram. To address this limitation and enable quantitative interpretation of the data, we developed an alternative elastocaloric protocol, which we refer to as the strong-coupling regime. In this regime, the sample temperature remains well thermalized to the platform while the measurement retains sensitivity to the strain-induced entropy response. This approach complements the conventional quasi-adiabatic elastocaloric limit and enables accurate thermodynamic extraction under mechanically constrained conditions.
Using ECE data measured in both the strong-coupling and quasi-adiabatic regimes as thermodynamic input, we reconstruct the absolute entropy landscape across the full temperature–strain phase diagram of Sr_2RuO_4. This combined approach exploits the absolute accuracy of low-frequency strong-coupling measurements together with the high signal-to-noise ratio of high-frequency quasi-adiabatic measurements. The resulting entropy map resolves the thermodynamic signatures associated with the stress-enhanced superconducting transition and enables the quantitative derivation of specific heat throughout the temperature–strain plane. The reconstructed heat capacity reveals no evidence for additional thermodynamically significant phase transitions within the superconducting dome and indicates an enhanced superconducting heat-capacity anomaly near the Van Hove point.

442	**Thickness Dependence of Transport Properties in Superconducting MgB_2 Thin Films**	Clemens Schmid	Contributed talk (17:00-17:15)

Clemens Schmid (1) Anton Pokusinskyi (2) Corentin Pfaff (3) Theo Courtois (3) Alexander Kasatkin (4) Karine Dumesnil (3) Stephane Mangin (3) Thomas Hauet (3) Oleksandr Dobrovolskiy (2)

(1) University of Vienna
(2) Technische Universität Braunschweig
(3) Université de Lorraine, Nancy, France
(4) G.V. Kurdyumov Institute for Metal Physics of the NAS of Ukraine, Kyiv, Ukraine

Magnesium diboride (MgB_2) is a superconductor with the highest critical temperature among conventional (electron-phonon) BCS-type superconductors at ambient pressure, making it a promising candidate for increasing the operating temperature of superconducting single-photon detectors [1]. The suitability of a material for such devices can be judged [2] via the maximal velocity of Abrikosov vortices in the film, inferred from the last voltage point before the abrupt transition to the highly resistive state associated with flux-flow instability (FFI). However, the high electron–electron scattering rate in MgB suppresses nonequilibrium phenomena near the critical temperature, making this assessment challenging.
In this work, we compare four gold-capped single-crystal MgB films with thicknesses between 12 and 45 nm. For all films we determine the pinning efficiency and critical current, both of which increase with film thickness. Measurements of the current–voltage characteristics for thinner films reveal multiple voltage jumps instead of a single FFI transition. We attribute this behaviour to the formation of regions with preferential vortex motion that evolve into normal domains [3]. This behaviour is supported by time-dependent Ginzburg-Landau modelling. For the 30 nm and 45 nm films, we observe single FFI transitions and extract vortex velocities up to 10–20 km/s. These values are the highest deduced for MgB_2 films so far and are comparable with the fastest vortex velocities recently found for other superconducting materials [4,5].

[1] J. Nagamatsu et al, Nature 410 (2001) 36.
[2] S.-Z. Lin et al, Phys. Rev. B 87 (2013) 184507.
[3] C. Schmid, A. Pokusinskyi, M. Gruber, C. Pfaff, T. Courtois, A. Kasatkin, K. Dumesnil, S. Mangin, T. Hauet and O. Dobrovolskiy, Crystal structure effects on vortex dynamics in superconducting MgB thin films, arXiv:2604.14022 (2026).
[4] L. Embon et al, Nat. Commun. 8 (2017) 85.
[5] O. Dobrovolskiy et al, Nat. Commun. 11 (2020) 3291.

302	**Superconductivity in Ni–Bi Bilayer Thin Films: Evidence for Anisotropic Strong-Coupling Pairing**	Sulagna Dutta	Contributed talk (17:15-17:30)

Sulagna Dutta (1) Vivas Bagwe (1) Pratap Raychaudhuri (1)

(1) Tata Institute of Fundamental Research, Mumbai

We report superconductivity in sputter-deposited Ni–Bi bilayer thin films with varying thicknesses [Bi (40–80 nm)/Ni (5–10 nm)]. While as-deposited films show no superconductivity, post-deposition annealing induces the formation of the intermetallic NiBi3 phase, leading to the emergence of superconductivity. The Bi (80 nm)/Ni (10 nm) film, corresponding closely to $NiBi_3$ stoichiometry, exhibits the sharpest transition with a maximum critical temperature ~4.16 K. The formation of the $NiBi_3$ phase is confirmed via XRD and EDX, establishing a direct correlation between superconductivity and phase formation. Transport measurements using four-probe resistivity and low-frequency two-coil mutual inductance techniques reveal sharp superconducting transitions.
Scanning tunneling microscopy and spectroscopy (STM/STS) were performed to investigate the microscopic nature of the superconducting state. Tunneling conductance spectra directly probing the quasiparticle density of states reveal a V-shaped gap structure with suppressed coherence peaks. The spectra are well described by anisotropic s-wave gap. The extracted gap value at 0.35mK is Δ(meV)=0.68 +0.3 cos(2θ), giving the maximum gap value to be 0.98meV. The corresponding gap ratio 2\Delta_{\mathrm{max}}/k_BT_c\approx5.5 is significantly larger than the weak-coupling BCS value of 3.53, demonstrating strong-coupling superconductivity. The temperature dependence of the superconducting gap \Delta(T), extracted from tunneling spectroscopy, clearly exhibits strong-coupling behavior. Zero-bias conductance maps under applied magnetic fields provide direct visualization of vortex states and their spatial distribution. From spatially resolved spectroscopy on the vortex core, the coherence length is estimated to be 23nm. We do not observe any signature of zero bias conductance peaks (ZBCP). Penetration depth measurements were performed in a 3He cryostat using a two-coil mutual inductance technique operating at 30 kHz. We obtain we get \lambda(T=0)\approx1.01\mu m for Bi 80 nm/Ni 10 nm film. The temperature variation of 1/\lambda^2 also indicates extremely strongly coupled superconductor.
Our study establishes NiBi3 as an anisotropic s-wave superconductor in the extremely strong coupling limit.

727	**Development of a Superconducting Bloch Transistor**	Rais Shaikhaidarov	Contributed talk (17:30-17:45)

Rais Shaikhaidarov (1) Ilya Antonov (1) Vladimir Antonov (1) Oleg Astafiev (1) Dmitry Golubev (2) Evgeni Il'ichev (3) Kyung Ho Kim (4) Sven Linzen (3)

(1) Royal Holloway University of London
(2) Aalto University
(3) Leibniz Institute of Photonic Technology
(4) Sejong University

The supercurrent quantization due to synchronization of the Bloch oscillations with microwaves in a small Josephson junction was recently demonstrated [1]. The current step is equal to 2efn, where 2e is Cooper pair charge, f is microwave frequency, and n is the integer. The effect is dual to the voltage quantization with step (h/2e)fn, the Shapiro steps, where (h/2e) is the superconducting flux quantum.

We use this phenomenon to develop a new quantum electronic device, the Bloch Transistor (BT). Its functionality is to deliver accurate current to the quantum circuit. One can vary the BT current by four controls: the bias and gate voltages, the frequency and amplitude of the microwave. The gate control of BT is promoted by the Aharonov-Casher effect [2]. The Bloch Transistor consists of two Josephson Junctions (JJ) connected in series, with small island between them. The Josephson junctions operate in a regime of the coherent quantum phase slip. This is provided by the choice of parameters of Josephson Junctions and the environment protection circuit, consisting of compact super-inductors and normal resistors. The flux tunnelling rate across the two junctions depends on the total charge of the island which is capacitively coupled to the gate electrode. The charge of the island controlled by the gate electrode potential.

1. Shaikhaidarov et al, Nature Comm., 15, 9326 (2024).
2. Y. Aharonov and A. Casher, Phys. Rev. Lett. 53, 319 (1984).

COND – Session 2 (Wed 23, 16:00-18:00)

ID	Title	Speaker	Type
94	**Structural reconstruction as the origin of the cuprate pseudogap**	Aline Ramires	Contributed talk (16:00-16:15)

Sophie Beck (1) Aline Ramires (1)

(1) TU Wien

High-temperature superconductivity in the cuprates emerges from an enigmatic metallic state, known as the pseudogap, characterized by a reconstructed Fermi surface, reduced carrier density, and the appearance of Fermi arcs, whose origin remains unresolved. Here, we show that these defining signatures naturally arise from a structural reconstruction observed experimentally that introduces a symmetry-enforced sublattice degree of freedom. In the presence of spin-orbit coupling, the Fermi surface is reconstructed into small closed pockets, effectively reducing the carrier density. The same sublattice structure gives rise to matrix-element interference in angle-resolved photoemission spectroscopy, leading to the manifestation of Fermi arcs. Density functional theory calculations support this mechanism. These results demonstrate that lattice symmetry provides a unifying and experimentally verifiable framework for understanding the pseudogap regime in the cuprates.

ID	Title	Speaker	Type
197	**Influence of Nesting on the performance of the Two-Particle Self-Consistent plus Dynamical Mean-field Theory Approach**	Xaver Christian Landerl	Contributed talk (16:15-16:30)

Xaver Christian Landerl (1)

(1) Technical University of Graz

We investigate the role of non-local electronic correlations in two-dimensional Hubbard models by combining and benchmarking complementary many-body approaches. In particular, we assess the performance of the two-particle self-consistent (TPSC) method and its extension with dynamical mean-field theory (DMFT), using cluster DMFT as a reference. To this end, we employ both continuous-time quantum Monte Carlo and a tensor-network-based fork tensor product state (FTPS) solver, the latter enabling direct access to real-frequency quantities and offering a potential route to cluster calculations without analytic continuation. We consider square-lattice systems with and without next-nearest-neighbour hopping, as well as the geometrically frustrated triangular lattice, thereby spanning regimes with varying degrees of nesting and frustration. For the square lattice, we find that the combined DMFT+TPSC approach reproduces cluster DMFT results with high accuracy at significantly reduced computational cost, while pure TPSC captures qualitative trends but exhibits deficiencies at low frequencies, particularly in the presence of strong nesting. On the triangular lattice, TPSC and DMFT+TPSC yield reasonable qualitative agreement with cluster results for non-local self-energies, though quantitative deviations persist. Our results demonstrate that DMFT+TPSC provides an efficient framework for incorporating short-range correlations beyond single-site DMFT, and highlight both the strengths and limitations of TPSC-based approaches across different lattice geometries.

ID	Title	Speaker	Type
596	**Microscopic mechanism and optical control of charge order in Kagome metals**	Yun Yen	Contributed talk (16:30-16:45)

Yun Yen (1) Fabio Caruso (2) Christoph Emeis (2) Michael Sentef (1)

(1) Institute for Theoretical Physics, Bremen Center for Computational Materials Science, University of Bremen, Bremen, Germany
(2) Institut fur Theoretische Physik und Astrophysik, Christian-Albrechts-Universitat zu Kiel, Kiel, Germany

Vanadium-based Kagome metals AV3Sb5(A = K, Rb, Cs) host competing charge density wave (CDW) states driven by enhanced correlations from van Hove singularities. These include Star-of-David and Tri-Hexagonal patterns, along with nematicity and possible time-reversal symmetry breaking, suggesting a loop-current order. These strongly competing phases make them promising for optical control, where photons can excite collective modes or manipulate ordered states.
However, the microscopic mechanism of the charge order—whether dominated by electron interactions or electron–phonon coupling--remains unclear. In this talk, we address this question using a Hartree–Fock mean-field approach based on an ab-initio model with electron–phonon couplings. We discuss how interaction form factors shape symmetry breaking across multiple free-energy minima, and study photoinduced dynamics with Ehrenfest dynamics. These results provide a microscopic basis for optical control of complex ordered states in Kagome metals.

ID	Title	Speaker	Type
244	**GQCA for the Mott Transition in Titanate/Vanadate Alloys**	Luka Wibmer	Contributed talk (16:45-17:00)

Luka Wibmer (1) Markus Aichhorn (1) Pedro Nunes Ferreira (1)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

The electronic configurations of the two perovskite-type transition metal oxides $SrTiO_3$ and $SrVO_3$ differ by only one electron, yet they exhibit drastically different electronic properties. $SrTiO_3$ is a band insulator, while $SrVO_3$ is a correlated metal. The substitutionally doped alloy of these materials $SrTi_{1-x}V_xO_3$ has thus seen increased interest over the last decades. Measurements of the alloy have shown a metal insulator transition (MIT) over its composition range. Previous supercell calculations have shown that this MIT is the result of local electron correlation effects, also called Mott physics, between the orbitals of

the material and suggest that the MIT may also depend on site disorder. In order to further investigate the MIT we use the generalized quasichemical approximation (GQCA) together with density functional theory and dynamical mean field theory (DFT+DMFT). With this approach, we can model the disordered alloy at every composition.
We show that GQCA together with DFT+DMFT can successfully be used on highly correlated alloys. Furthermore, we model the MIT in $SrTi_{1-x}V_xO_3$ over the entire composition range using ab-initio methods.

340	**Evolution of Electronic, and Magnetic Properties of Intercalated 2H-NbS_2 and 2H-TaS_2**	Gaurav Pransu	Contributed talk (17:00-17:15)

Gaurav Pransu (1) Neven Barišić (2) Yuki Utsumi Boucher (1) Naveen Dhami (3) Bruno Gudac (1) Mirta Herak (1) Mario Novak (1) Petar Popčević (1) Wojciech Sas (4)

(1) Physics Department, Faculty of Science, University of Zagreb, Zagreb, Croatia
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(4) Institute of Nuclear Physics, Polish Academy of Sciences, Kraków, Poland

Transition metal dichalcogenides (TMDs) are a layered class of materials known for their rich physical properties, including charge density waves (CDWs) and superconductivity. Their layered crystal structure allows for the intercalation of first-row transition metals into the van der Waals gaps, which significantly modifies the physical properties of the host material, suppressing CDW and superconducting ground states while inducing magnetic order and enabling potential applications in spintronics and novel electronics [1].
In this study, we synthesized high-quality single crystals of NixNbS2 across a broad intercalation range (0.01 < x < 0.6), as well as stoichiometric Co1/3TaS2. Both systems exhibit antiferromagnetic ordering; however, a measurable ferromagnetic component was also observed in each, indicating the presence of Dzyaloshinskii–Moriya interactions.
We investigated the influence of intercalation on the electronic structure, magnetic and transport properties using angle-resolved photoemission spectroscopy (ARPES) and magnetotransport measurements [2]. Ongoing work involves applying both uniaxial and hydrostatic pressure to further understand the coupling between the metallic and magnetic subsystems [3].

[1] R. H. Friend et al., Adv. Phys. 36 (1987) 1–94.
[2] Y. U. Boucher et al., Phys. Rev. B 109 (2024) 085135.
[3] P. Popčević et al., Phys. Rev. B 107 (2023) 235149.

165	**Dual-Ion Magneto-Ionics in Nanoporous $Pd_{75}Co_{25}$ Alloy**	Stefan Eber	Contributed talk (17:15-17:30)

Stefan Eber (1) Georg Haberfehlner (2) Peter Banzer (3) Roland Würschum (1) Stefan Topolovec (1)

(1) Institute of Materials Physics, Graz University of Technology
(2) Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology
(3) Institute of Physics, University of Graz

Magneto-ionics is an approach that enables the energy-efficient tuning of magnetic properties by electrochemical charging. Materials with a high surface-to-volume ratio are particularly suitable for this purpose. In the present work [1], we prepared a nanoporous Pd75Co25 alloy by dealloying the precursor Al80(Pd75Co25)20, achieving pore sizes in the range of 10 nm.
In-situ SQUID magnetometry, in combination with a detailed electrochemical analysis, reveals that the reversible reduction/formation of surface-based Co oxides and hydroxides leads to substantial variations in the magnetization. In fact, a switching between a weakly magnetic OFF state, and a ferromagnetic ON state, characterized by a significantly enhanced saturation magnetization, can be achieved using this voltage-triggered electrochemical reaction. Furthermore, with specific electrochemical measurement techniques, a second, smaller magneto-ionic effect based on the absorption/desorption of hydrogen was observed in the same alloy.
Ongoing experiments focus on investigating the behavior of both magneto-ionic effects in Pd-Co alloys of varying compositions.

[1] S. Eber et al., ACS Mater. Au., 2026, in press. (DOI: 10.1021/acsmaterialsau.5c00245)

304	**Investigation of Spin-Polaron Breakdown in the Single-Hole Doped Two-Dimensional t-t'-Jz Model**	Matthias Bernhart	Contributed talk (17:30-17:45)

Matthias Bernhart (1) Jiri Chaloupka (2) Alessandro Toschi Krzysztof Wohlfeld (3)

(1) Institute of Information Systems Engineering and Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria
(2) Masaryk University, Department of Condensed Matter Physics
(3) University of Warsaw

Originating from Fermi liquid theory, the quasiparticle concept is the fundamental workhorse of solid-state physics. However, while it describes many-body systems in many materials, it fails to account for the exotic phases emerging from strong electronic correlations. We investigate the stability of the spin polaron quasiparticle by examining the 2D $t - J^z$ model and introducing a next-nearest-neighbor hopping t', which results in the $t - t' - J^z$ model. Using an exact diagonalization approach based on ARPACK, we solved single-hole doped systems in the antiferromagnetic regime with a fixed Ising coupling of $J^z = 0.4t$ and varied t' from $-0.5t$ to $0.5t$. We performed a finite-size scaling analysis of the quasiparticle weight at the Γ-point and X-point for lattices of up to 32 sites. Extrapolation toward the thermodynamic limit reveals an "anomalous" regime at the Γ-point for $t' \leq -0.3t$, characterized by a vanishing quasiparticle weight. To characterize the low-energy dynamics within this regime ($t' \leq -0.3t$), we evaluated the spin correlations centered around the hole and the magnon number distribution on a 20-site lattice. Based on these results, we propose a preliminary picture of the single-hole doped antiferromagnetic ground state within the "anomalous" regime. This state deviates from the well-known spin polaron because the cloud of magnetic fluctuations, typically localized around the hole, delocalizes over the whole finite-size lattice. Consequently, such systems show a weakly suppressed antiferromagnetic configuration under single-hole doping.

122	**Topological Hall Response from Canted Antiferromagnetic Order in d- Electron Kagome Systems**	Waquar Ahmed	Contributed talk (17:45-18:00)

Waquar Ahmed (1) Roland Hayn (1) Steffen Schäfer (1) Pierre Lombardo (1) Imam Makhfudz (1)

(1) Aix Marseille University

In a *d*-electron system on a kagome lattice, a non-trivial intrinsic Berry curvature may arise from the interaction with a non-collinear antiferromagnetic spin order. This opens the route for a quantum anomalous Hall effect in the multi-orbital system, even without an external magnetic field, explicit spin-orbit coupling or relativistic effects. For spin orders with an out-of-plane component, the scalar spin chirality is finite, and the integration of the Berry curvature over the Brillouin zone may yield integer Hall conductivities in units of e^2/h. For a Fermi level within a nontrivial gap, the canted configuration offers, at least in principle, the posibility for a maximal Chern number, $C = \pm 5$. Candidate materials are considered in this paper. In existing materials, the electron hopping is generally highly anisotropic, leading to a quantum anomalous Hall effect with smaller Chern numbers. A topological phase transition between Hall plateaus of opposite can be driven by flipping the out-of-plane component of the spin order, alluding to the potential of this system to applications in quantum information.

COND – Session 3 (Thu 24, 16:00-18:00)			
ID	Title	Speaker	Type
292	Entanglement Structures in Topological Phases of Matter	Bishal Kumar Ghosh	Contributed talk (16:00-16:15)

Bishal Kumar Ghosh (1) Viktor Eisler (1)

(1) Department of Physics, Univrsity of Graz

Real-space entanglement encodes key information about topological order in many-body systems. Our work aims to target quantum Hall systems, focusing on the entanglement Hamiltonian (EH), which gives the total characterization of entanglement between a subsystem and its environment. In particular, we study the EH for the integer quantum Hall system and show that, for each angular momentum sector, it can be accurately described by a deformation of the physical Hamiltonian with position-dependent prefactors. We demonstrate how this ansatz can provide an approximation of the entanglement entropy and also test the limits at which it fails to do so. Our results provide novel insight into the entanglement properties of gapped two-dimensional electron systems.

386	**Highly Excited 2DEG in a Driven Cylindrical FIR-Photon Cavity**	Wen-Hsuan Kuan	Contributed talk (16:15-16:30)

Wen-Hsuan Kuan (1) Vidar Gudmundsson (2,3) Andrei Manolescu (3)

(1) Department of Applied Physics and Chemistry, University of Taipei, Taipei 10048, Taiwan
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(3) Department of Engineering, Reykjavik University, Menntavegur 1, IS-102 Reykjavik, Iceland

The present work examines light-matter interactions in a two-dimensional electron gas formed in a periodic lateral superlattice, subjected to a perpendicular homogeneous magnetic field, and embedded in a cylindrical far-infrared photon cavity. The electronic states are constructed in the magneto-translational invariant Ferrari basis, which naturally captures the magnetic Bloch structure of the system. Within this framework, photon replicas, as well as para- and diamagnetic contributions to the coupled electron-photon dynamics, are treated on equal footing.
The calculations are carried out using a quantum electrodynamics density functional theory (QED-DFT) approach combined with a tensor-product (TP) representation of electron and photon states. While electron-electron interactions are incorporated at the level of QED-DFT, the electron-photon coupling is treated nonperturbatively via exact diagonalization (configuration interaction) within each self-consistent iteration. This allows for a consistent description of photon-dressed electronic states and their dynamical response.
The coherent dynamics provides a controlled setting to identify resonant and off-resonant excitation regimes, which are essential for application to open-system descriptions where environmental coupling and relaxation processes are included.
The results reveal a clear distinction between resonant and off-resonant driving conditions. In the near-resonant regime, the system exhibits a pronounced and sustained increase in total energy and photon occupation, indicating efficient energy transfer from the external drive into photon-dressed collective modes. In contrast, for detuned excitation, the dynamics remain bounded and are characterized by coherent oscillations with pronounced beating patterns, reflecting reversible energy exchange between the electronic and photonic degrees of freedom.
These observations suggest that detuning plays a critical role in controlling the long-time dynamics of the driven system. Off-resonant driving suppresses sustained energy accumulation and stabilizes the dynamics, leading to behavior that qualitatively resembles a weakly dissipative response. This highlights the importance of frequency and phase matching between the external drive and the underlying photon-dressed excitation spectrum, and provides a physically transparent reference for assessing the impact of dissipation in open-system extensions.

47	**Angular-momentum-selective nanofocusing with Weyl semimetals**	Marco Peluso	Contributed talk (16:30-16:45)

Marco Peluso (1) Alessandro De Martino (1) Reinhold Egger (2) Francesco Buccheri (1)

(1) Politecnico di Torino
(2) Heinrich-Heine-Universität, Düsseldorf

Surface plasmon polaritons enable the confinement and manipulation of electromagnetic radiation far below the diffraction limit and constitute a key platform for nanoscale photonics. In conventional plasmonic systems, however, nanofocusing on tapered metallic structures is strongly constrained by the plasmonic dispersion. In particular, for conical metallic tips typically only a single mode can propagate towards the apex, limiting the control of additional photonic degrees of freedom such as orbital angular momentum. Here we investigate theoretically the propagation of surface plasmon polaritons on a conical tip made of a magnetic Weyl semimetal. The nontrivial topological band structure of Weyl semimetals, characterised by the presence of Weyl nodes, gives rise to a modified electromagnetic response that alters the propagation of plasmonic modes. As a consequence, all modes with a given sign of orbital angular momentum can propagate towards the tip apex and be nanofocused. These results reveal a mechanism for angular-momentum-selective plasmonic nanofocusing and highlight the potential of topological materials for manipulating structured light at the nanoscale.

668	**Topological markers for a one-dimensional fermionic chain coupled to a single-mode cavity**	Anna Ritz-Zwilling	Contributed talk (16:45-17:00)

Olesia Dmytruk (1) Anna Ritz-Zwilling (1)

(1) CPHT, CNRS, Ecole polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

We study a Su-Schrieffer-Heeger chain coupled to a single mode photonic cavity. Considering an off-resonant regime we use the high-frequency expansion in order to obtain an effective fermionic Hamiltonian with cavity-mediated interactions. We characterize the effects of the cavity on topology in a finite size chain by studying three different markers adapted for interacting systems: correlation functions between edges in a chain with open boundary conditions, and a winding number based on the single-particle Green's function and bulk electric polarization via the many-body formula by Resta for a chain with periodic boundary conditions. There is excellent agreement between the winding number and polarization approaches to compute the phase diagram, with the presence of the edge states being confirmed through the calculations of the two-point correlation function. Our approach provides an alternative perspective on cavity-modified topological phases through a study of an effective interacting electronic Hamiltonian and complements methods that treat the full light–matter Hamiltonian directly.

A. Ritz-Zwilling and O. Dmytruk, arXiv:2604.13936 (2026)

497	**Semiclassical Wave-Packet Dynamics: Quantum-Metric Effects**	Luca Maranzana	Contributed talk (17:00-17:15)

Luca Maranzana (1) Koki Shinada (2) Ying-Ming Xie (2) Sergey Artyukhin (1) Naoto Nagaosa (2)

(1) Italian Institute of Technology
(2) RIKEN Center for Emergent Matter Science

Quantum geometry governs a wide range of transport and optical phenomena in quantum materials. Recent works have explored analogue electromagnetism and gravity in terms of the quantum geometric tensor, whose real and imaginary parts correspond to the quantum metric and the Berry curvature. By treating real- and momentum-space geometries on an equal footing, we develop a comprehensive and general formalism based on an expansion in $\hbar$, equivalent to an expansion in spatial derivatives. We derive the quantum-metric corrections to the wave-packet energy, the Berry connection, and the phase-space density of states, similar to the field-induced corrections in nonlinear response. A kinetic equation that captures quantum-metric effects across the full phase space then follows naturally. We further identify a polarization induced by gradients of the metric and a linear Hall response originating from its mixed components. Our framework provides a foundation for investigating thermodynamic and transport properties in systems where real- and momentum-space quantum geometries coexist.

556	**Observation of the Charge Density Wave Excitonic Order Parameter in Topological Insulator Monolayer WTe_2**	Iolanda Di Bernardo	Contributed talk (17:15-17:30)

Yang-Hao Chan (1) Iolanda Di Bernardo (2) Mark Edmonds (3) Michael Fuhrer (3) Manuela Garnica (4) Amit Kumar (5) Amadeo L. Vazquez de Parga (2) Hsin Lin (6) Shantanu Mukherjee (7) Michal Papaj (8) Yande Que (5) Joan Ripoll-Sau (2) Zhengjue Tong (5) Liam Watson (3) Bent Weber (5)

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(8) Department of Physics, University of Houston, Houston, Texas 77204, United States

Strong electron–hole interactions in a semimetal or narrow-gap semiconductor may drive a ground state of condensed excitons. Monolayer WTe_2 has been proposed as a host material for such an exciton condensate, but the order parameter–the key signature of a macroscopic quantum-coherent condensate–has not been observed. Here, we use Fourier-transform scanning tunneling spectroscopy (FT-STS) to study quasiparticle interference (QPI) and periodic modulations of the local density of states (LDOS) in monolayer WTe_2. In WTe_2 on graphene, in which the carrier density can be varied via back-gating, FT-STS shows QPI features in the two-dimensional (2D) bulk bands, confirming the interacting nature of the bandgap in neutral WTe_2 and the semimetallic nature of highly n- and p-doped WTe_2. We observe additional nondispersive spatial modulations in the LDOS imprinted on the topological edge mode of neutral WTe_2 on metallic substrates (graphene and graphite), which we interpret as the interaction of the topological edge mode with the expected charge density wave order parameter of the excitonic condensate in WTe_2 at low interaction strength due to screening by the metallic substrates.

275	**From Solutions to Plasmonic Nanostructures: a Quantum Embedding Framework for Molecular Response Properties**	Alberto Barlini	Contributed talk (17:30-17:45)

Alberto Barlini (1) Tommaso Giovannini (2)

(1) Scuola Normale Superiore
(2) University of Rome Tor Vergata

Molecular response properties are central to the interpretation and design of functional systems for photonics, sensing, and nonlinear optical applications, yet their accurate description in the condensed phase remains challenging.[1–4] In such complex systems, the target molecule interacts with an environment ranging from transparent media, such as liquid solutions, to nanostructured substrates, such as metal nanoparticles.[1–4,6,8] A convenient route to address this complexity is to resort to quantum embedding methods, in which the full system is partitioned into interacting subsystems, allowing the region of primary interest to be treated at a high quantum-mechanical level while retaining an efficient and physically consistent description of the environment.[2–5,7] In solvated systems, the external radiation mainly interacts with the solute, while the external medium modifies the response through electrostatic, polarization, and short-range quantum effects.[1,3,4,8] In contrast, metal nanoparticles can absorb the electromagnetic radiation yielding to the collective excitation of localized surface plasmons, which strongly enhance the local field at the surface, and substantially modifying the electronic structure of molecular adsorbates.[6,8]

In this contribution, we present an integrated quantum-embedding/classical framework for molecular response properties in complex environments, ranging from solutions to nanostructured materials within a unified formalism.[3–8] The approach is based on multilevel density functional theory (MLDFT), in which the system is partitioned into active and inactive quantum subsystems described at the DFT level, to response theory through coupled-perturbed Kohn-Sham equations for the MLDFT Hamiltonian.[5,7] We showcase the accuracy of the approach for selected systems in solution, and we discuss the challenges for accurately describing hybrid molecule-plasmons systems, especially surface-enhanced spectral response.[4,6,8]

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[3] Giovannini, T; Egidi, F; Cappelli, C. Chem. Soc. Rev. 2020, 49, 5664-5677.
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COND – Session 4 (Fri 25, 10:30-12:30)

ID	Title	Speaker	Type
459	**Elucidating the Origin of Guest-Induced Phase Transformations in a Flexible Metal-Organic Framework Through Experiment and Theory**	Peter Hartmann	Contributed talk (10:30-10:45)

Peter Hartmann (1)

(1) University of Graz

Flexible metal-organic frameworks (MOFs) are at the forefront of energy storage research due to their ability to undergo structural transformations triggered by guest molecule uptake.[1-4] However, controlling phase formation and uncovering the nanoscopic mechanisms governing these transformations remain major challenges.
In this work, we provide a comprehensive investigation of how azobenzene acts as a guest molecule to influence the crystal phase stabilization of DMOF-1 and, more broadly, demonstrate that guest-host interactions play a decisive role in directing the final phase formation. Combining computational simulations with in-situ and ex-situ X-ray scattering and UV-Vis spectroscopy, we reveal how experimental conditions govern the transformation pathway, leading to either open-pore/large-pore or narrow-pore DMOF-1 structures incorporating azobenzene within the pores. Solid-state density functional theory (DFT) calculations further clarify how the arrangement of azobenzene molecules modulates phase stability and quantify the corresponding stored energy through Helmholtz free energy profiles.
This integrated computational-experimental approach establishes a general framework linking preparative conditions and guest-host interactions to phase behavior, enabling the rational design of flexible MOF-based phase-change materials for energy storage applications.

[1] Griffiths, K. et al., Crystal growth & design, 23, 7044–7052 (2023).
[2] Yanai, N. et al., Journal of the American Chemical Society, 134, 4501–4504 (2012).
[3] Klokic, S. et al., Nature Communications, 16, 7135 (2025).

ID	Title	Speaker	Type
621	**Discovery of Sustainable Energy Materials via the Machine-Learned Material Space**	Erich Runge	Contributed talk (10:45-11:00)

Erich Runge (1) Malte Grunert (1) Max Großmann (1)

(1) TU Ilmenau

Does a machine learning (ML) model capture the intrinsic structure of the material space? The example of the OptiMate model, a graph attention network trained to predict the optical properties of semiconductors and insulators, provides an affirmative answer. By applying the UMAP dimensionality reduction technique to its latent embeddings, it is demonstrated that the model captures a nuanced and interpretable representation of the materials space, reflecting chemical and physical principles, without any user-induced bias. This enables clustering of almost 10,000 materials based on optical properties and chemical similarities. Furthermore, it is shown how the learned material space can be used to identify more sustainable alternatives to critical materials in energy-related technologies, such as photovoltaics. These findings demonstrate the dual utility of ML models in materials science: Accurately predicting material properties while providing insights into the underlying materials space. The approach demonstrates the broader potential of leveraging learned materials spaces for the discovery and design of materials for diverse applications, and is easily applicable to any state-of-the-art ML model.

M. Grunert, M. Grossmann, E. Runge: Nat. Commun. 16, 8142 (2025), Small 22, 2412519 (2026), Appl. Phys. Lett. 128, 053302 (2026)

ID	Title	Speaker	Type
34	**Strain engineering quantum properties on 2D materials**	Reyes Calvo	Contributed talk (11:00-11:15)

Reyes Calvo (1)

(1) BCMaterials

Since the discovery of graphene, two-dimensional (2D) materials with different properties—ranging from semiconductors to superconductors and magnets—have been isolated. A defining characteristic of these materials is their sensitivity to external perturbations, which makes them highly tunable. Strain engineering is a powerful tool that leverages the mechanical flexibility of 2D materials to modulate their electronic, optical, and magnetic responses.

While the tuning of semiconducting properties has been extensively explored at room temperature, strain effects on quantum phenomena—including superconductivity and magnetism—remain comparatively unexplored, despite strong theoretical predictions suggesting that strain can modulate or even induce emergent phase transitions. This is partially due to the lack of suitable methods to apply controlled strain in 2D materials at low temperatures, where many of these quantum phenomena emerge.
In this talk, I will present a series of recent experiments that overcome these challenges by using thermal mismatch with polymeric substrates to induce uniform, biaxial compressive strain in 2D crystals under cryogenic conditions. This approach enables a robust strain-driven modulation of quantum phenomena across different material systems. I will show how strain can be used to tune neutral and charged excitons in monolayer transition metal dichalcogenides [1], shift the superconducting transition in few-layer $NbSe_2$ [2], and enhance magnetoresistance and magnetic anisotropy in the antiferromagnetic semiconductor CrSBr [3]. Our approach provides a straightforward method to tune and control phase transitions and quantum properties in 2D materials at cryogenic temperatures. Our findings highlight the potential of strain engineering to adjust the properties of 2D materials for spintronics and quantum technology applications.

[1] E. Henriquez-Guerra et al., Large Biaxial Compressive Strain Tuning of Neutral and Charged Excitons in Single-Layer Transition Metal Dichalcogenides, ACS Applied Materials & Interfaces 2023 15 (49), 57369-57378.
[2] E. Henriquez-Guerra et al. Modulation of the Superconducting Phase Transition in Multilayer 2H-NbSe2 Induced by Uniform Biaxial Compressive Strain Nano Letters 2024 24 (34), 10504-10509
[3] E. Henriquez-Guerra et al. Strain Engineering of Magnetoresistance and Magnetic Anisotropy in CrSBr. Advanced Materials 2025, 2506695.

278	**Temperature-modulated dilatometry as a tool for studying precipitation kinetics in alloys**	Marcel Simhofer	Contributed talk (11:15-11:30)

Marcel Simhofer (1) Philipp Brunner (1) Jiehua Li (2) Wolfgang Sprengel (1) Roland Würschum (1)

(1) TU Graz
(2) Montanuniversität Leoben

Temperature-modulated dilatometry represents a powerful technique for studying kinetic processes in materials, such as, e.g., the equilibration of the concentration of thermally formed lattice vacancies in metals [1]. In the present work, the application potentials of this technique are explored with respect to precipitation kinetics in alloys. Al-Mg is used as case example, where the phase equilibration between the saturated solid solution Al(Mg) and the intermetallic Al3Mg2 phase is monitored [2]. Upon temperature modulation, the variation of relative phase fractions, which arises from the temperature-dependent Mg-solubility in Al, can be specifically detected by dilatometry due to the different atomic volumes of the intermetallic phase and the solid solution. The equilibration process causes a phase shift between the periodic length change and the applied sinusoidal temperature modulation, which gives access to the underlying kinetic processes. The measured variation of the phase shift with the modulation frequency is quantitatively analyzed in the framework of a simple kinetic model, revealing that the equilibration process is controlled by the diffusion of Mg in Al.

[1] R. Würschum et al., Int. J. Mater. Res. 113 (2022) 683.
[2] M. Simhofer et al., J.Alloys&Comp. 1010 (2025) 176984.

523	**Materials discovery with ephemeral data derived potentials**	Peter Cooke	Contributed talk (11:30-11:45)

Peter Cooke (1) Chris J. Pickard (1)

(1) University of Cambridge

The development of machine learned interatomic potentials (MLIPs) has revolutionised atomistic simulations over recent years. MLIPs enable simulations with accuracy comparable to quantum mechanical approaches at up to 10 million times smaller computational cost. The ephemeral data derived potentials (EDDPs) are a flexible class of MLIP that can utilize comparatively small neural networks for fast and accurate simulations. Materials discovery techniques, such as random structure searching, can exploit this acceleration in a number of ways. Larger system sizes and chemical spaces can be explored, or more computationally intensive structure optimizers, utilizing molecular dynamics, can be incorporated. Through a range of applications, we demonstrate that more complex optimizers can improve search performance for large systems. Through example simulations in LAMMPS, we further show that EDDPs can be employed beyond structure searching, to explore complex dynamical behaviour and synthesis pathways across a range of conditions and chemical systems.

367	**Numerical Study of Randomness-Induced Rounding of a First-Order Phase Transition in Liquid-Crystal Models**	Rei Amano	Contributed talk (11:45-12:00)

Rei Amano (1) Takeaki Araki (1)

(1) Department of Physics, Kyoto University

First-order phase transitions are known to be suppressed by arbitrarily weak quenched disorder in two-dimensional and lower systems, a phenomenon referred to as the rounding effect. In three-dimensional systems, numerical studies have reported similar behavior in discrete models, although a finite disorder strength is required. In contrast, evidence for this effect in three-dimensional continuous systems remains limited.
Motivated by experimental observations that the first-order isotropic–nematic (I–N) transition disappears in rod-like micellar systems under certain conditions, we investigate Lebwohl-Lasher liquid-crystal models with randomized interaction coefficients and extended higher-order orientational couplings, serving as representative three-dimensional continuous random-bond systems. The Hamiltonian is given by $-\sum_{<i,j>} J_{ij}\left(s_i \cdot s_j\right)^p$, where $J_{ij} = J_i \times J_j$ with random variables J_i drawn from $\mathcal{N}(J_0, J^2)$, and p is an even positive integer. As a measure of the randomness, we use $J'^2 := \mathrm{Var}[J_{ij}]$. Using Metropolis and Wang-Landau algorithms, we examine the emergence of the rounding effect and characterize its properties.
We provide numerical evidence for the occurrence of the rounding effect in three-dimensional liquid-crystal systems and demonstrate the existence of a finite disorder threshold J'_c, consistent with previous results for discrete models. Furthermore, our results suggest that under sufficiently strong disorder, the system may enter a regime that cannot be straightforwardly described within the conventional second-order transition framework. We also discuss the influence of different probability distributions of random interactions on the I–N phase transition.

410	**Breakdown of linear response in the recoil dynamics of a colloid in viscoelastic media**	Jose Rafael Bordin	Contributed talk (12:00-12:15)

José Rafael Bordin (1) Matthias Fuchs (2)

(1) Universidade Federal de Pelotas, Brasil
(2) Universität Konstanz, Germany

Understanding the microscopic response of complex fluids to localized perturbations is a central problem in soft condensed matter. Here, we investigate the dynamics of a colloidal probe driven through a viscoelastic medium composed of interacting polymer chains using Langevin dynamics simulations.
Recent experimental protocols have provided direct access to stored elastic forces in such systems. In these experiments, a colloidal probe is driven either at constant force or constant velocity and, upon release, exhibits a recoil motion. This back-motion reflects memory effects in the viscoelastic medium and encodes information about its relaxation dynamics.
Motivated by this approach, we analyze the recoil of the probe after switching off the external driving. By tuning the strength of polymer–polymer interactions, we control the viscoelastic character of the medium, ranging from purely repulsive to increasingly adhesive systems. Our results reveal a nontrivial dependence of the recoil on both the driving protocol and interaction strength. In weakly interacting systems, the recoil is reasonably described by linear response theory at intermediate forces, while deviations emerge at low forcing. For intermediate adhesion, we observe enhanced recoil and subdiffusive dynamics, indicating strong memory effects and persistent correlations. At higher adhesion, particle motion becomes increasingly constrained, leading to reduced recoil despite increased structural rigidity.
These findings highlight the interplay between microscopic interactions, memory, and nonlinear response in viscoelastic media, providing a minimal framework to interpret active microrheology experiments.

COND – Posters (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
701 **P083**	**Fast Many-Body Total Energy Calculations Using Approximate Impurity Solvers in DFT+DMFT**	Michael Stadtmann	Poster

Markus Aichhorn (1) Michael Stadtmann (1)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

Accurate total energy calculations within the combined Density Functional Theory and Dynamical Mean-Field Theory (DFT+DMFT) framework are essential for predictive studies of correlated materials, but remain computationally demanding when using numerically exact impurity solvers such as continuous-time quantum Monte Carlo (CT-QMC). This limitation is particularly severe for problems involving structural degrees of freedom such as volume optimization or lattice distortions in correlated materials where repeated total energy evaluations are required.
In this work, we explore the use of approximate impurity solvers to significantly accelerate many-body total energy calculations. In particular, we employ an exact diagonalization (ED) solver based on the EDIpack library and assess its performance against CT-QMC benchmarks. Using $SrVO_3$ as a prototypical correlated metal, we perform a systematic comparison of total energies and including calculations as a function of unit cell volume.
We show that, despite its approximate nature due to bath discretization, the ED solver can in particular cases achieve close agreement with CT-QMC results when an appropriate bath parametrization is employed, while computational costs are reduced by orders of magnitude. This efficiency makes ED-based approaches particularly well suited for structural optimization and the study of correlation-driven lattice effects, including Jahn-Teller distortions in perovskites.
Our results demonstrate that approximate solvers, when carefully implemented, provide a reliable and efficient route for many-body total energy calculations within DFT+DMFT, enabling scalable studies of structurally complex correlated systems.

ID	Title	Presenter	Type
282 **P084**	**Unveiling Topology with Non-Linear Hall Effect**	Helena Silva	Poster

Helena Silva (1) André M. Pereira (1) Vítor M. Pereira (1)

(1) University of Porto

The Non-Linear Hall Effect (NLHE) represents a novel class of Hall-like phenomena that emerge without the need for time-reversal symmetry breaking, distinguishing it from conventional Hall effects. It consists of a transverse electric response which has a second-order contribution on the applied longitudinal current and arises from both intrinsic and extrinsic contributions. The intrinsic contribution is connected to the Berry curvature dipole (BCD), while the extrinsic contribution arises from the scattering sources in the system.
This study explores how this second-order response manifests in time-reversal invariant and inversion-breaking materials when subjected to an external electric field. Using semiclassical Boltzmann transport theory within the framework of the tilted 2D massive Dirac model, we investigate the influence of impurity scattering and electron–phonon interactions, allowing us to study the effect of temperature variation. To establish a realistic physical origin for the tilt parameter, we derive the effect of uniaxial strain within a tight-binding framework and show that strain can effectively be interpreted as a tilt parameter in the low-energy Dirac Hamiltonian. Different strain percentages are considered to evaluate how experimentally accessible strain conditions can modify the electronic structure and influence the NLHE.
Experimentally, a modified conventional Hall setup with an AC current and lock-in amplifiers is employed to study Bi_2Se_3 samples. This study opens new pathways for investigating the topological and symmetry properties of emergent quantum materials.

ID	Title	Presenter	Type
510 **P085**	**Multi-orbital physics in inverse Lieb lattice altermagnets**	Jannik Gondolf	Poster

Mercè Roig (1) Jannik Gondolf (2) Andreas Kreisel (3) Brian Moller Andersen (2) Daniel Agterberg (1)

(1) University of Wisconsin-Milwaukee
(2) Niels Bohr Institute, University of Copenhagen
(3) Uppsala University

The Lieb lattice is a promising framework for d-wave altermagnetic material candidates. We explore the physics arising from multiple orbitals present at the Fermi level and the consequences for stabilizing altermagnetism on the Lieb lattice by deriving microscopic tight-binding models for different orbitals. We show that for vanadium oxichalcogenide candidate materials with d_{xy} and $d_{xz/yz}$ orbitals at the Fermi level, the d_{xy} orbital is crucial to stabilize the

altermagnetic order, and the $d_{xz/yz}$ orbital becomes altermagnetic through coupling. We further study implications for potential topological states in the presence of spin-orbit coupling.

298 **P086**	**Optimal Local Orbitals: A Systematic Approach for Accurate Wavefunction Representation**	Ann Chantal Goutier	Poster

Ann Chantal Goutier (1) Michael Schüler (1)

(1) Paul Scherrer Institut

Electronic structure calculations in solids are commonly performed in large plane wave or real space basis sets. These basis sets are compressed and localised around atoms for advanced postprocessing, such as calculations of the Berry curvature or optical properties. For this purpose, most commonly one constructs Maximally Localised Wannier Functions (MLWFs). MLWFs are constructed to preserve the band structure for some low-energy bands exactly, but may not yield accurate results for properties requiring the explicit calculation of the corresponding wave function.
We instead propose a method for a wave function based scheme for Hamiltonian compression. We started from optimised Atomic Orbitals(AOs) and generate optimal Local Orbitals (LOs) by optimising a projectability operator variationally, using algorithmic differentiation. We disallowed mixing between orbitals of different atoms for the optimisation to preserve the localised nature of our orbitals. We included an iterative improvement of a projectability-based disentanglement. This approach requires little information about the system and is therefore compatible with high throughput calculations. It also allows for systematic improvement by increasing the number of LOs.
We also used schemes to improve the interpolation of the band structure in local orbital space, such as a Loewdin correction to the Hamiltonian or a k point dependent mixing of the LOs based on the principle of Intrinsic Atomic Orbitals.
Finally, we showcase the potential of using such a compressed basis set in calculating optical properties using the example of dipole operator calculations.

72 **P087**	**Directed autonomous motion of active Janus particles induced by wall-particle alignment interactions**	Poulami Bag	Poster

Poulami Bag (1)

(1) Presidency University

Active particles confined in narrow channels often explore high dimensional phase spaces where symmetry breaking mechanisms can give rise to directed transport. These particles possess persistent motion which arises from continuous conversion of energy into self-propulsion. Although this directed motion becomes inefficient in long times due to the effects of thermal and rotational diffusion, leading to random particle trajectories. Therefore, to suitably tailor active particle dynamics for practical applications, efficient methods are required to achieve directed motion. In this work we present a highly efficient mechanism based of particle-wall alignment interaction for rectification of particle transport. Using numerical simulations we show that a subtle asymmetry in strength of interaction between the opposite channel walls with particle or a gravitational bias is sufficient to break the inversion symmetry and generate directed motion of chiral active micro-swimmers with over 60% efficiency. Here, chirality refers to the presence of intrinsic angular velocity, resulting in circular trajectories in either clockwise or anti-clockwise direction along with translational motion. For achiral active particles, rectification happens only in presence an unbiased external fluid flow that perturbs the particle dynamics and introduce orbiting motion. Thus, we put achiral particles inside Couette flow to break the upside down symmetry and exhibit spontaneous directed motion. Further we have checked the robustness of rectification by our proposed method against various self-propulsion properties, particle's intrinsic chirality and several stable velocity orientations of the particle with respect to channel walls. We believe our findings offer deep insights to gear motion of artificial as well as natural active systems.

39 **P088**	**Field free Josephson diode effect using unconventional magnets**	Lovy Sharma	Poster

Lovy Sharma (1)

(1) Indian Institute of Technology Delhi, New Delhi

The p-n junction diode is a cornerstone of electronics, but its rectification is intrinsically dissipative. Recently, its superconducting analogue, the Josephson diode effect (JDE), characterised by unequal critical currents in opposite directions in Josephson junction (JJ), has been observed experimentally and predicted theoretically in models of planar JJs. Realising JDE typically requires breaking both time reversal and inversion symmetry, which is often implemented using external magnetic field or incorporating ferromagnetic materials. However, these approaches introduce stray fields and magnetic cross-talk, posing a significant obstacle for device integration.\
Here we establish a field-free route using unconventional magnets namely, altermagnet \cite{reference1} and p-wave magnet \cite{reference2}. These magnets break time reversal symmetry (TRS) while maintaining zero magnetisation. We demonstrate that the mere breaking of time-reversal and inversion symmetry is not sufficient to guarantee a diode effect. We have provided necessary conditions for the diode effect using altermagnet as barrier in JJ without using external field. The diode effect is also shown to be tunable using gate potential, change polarity and increasing non-reciprocity, offering a simple experimental knob for control.
Using p-magnet in proximity s-wave SC as the leads of JJ, with AM as barrier we also shown that we do not require Rashba SOC, which was emphasised in previous theoretical proposals. Moreover in both type of junction the efficiency of diode effect is reached about 45%.

577 **P089**	**Quasi 2D altermagnets and multi-ferroic altermagnets $BiFeO_3$**	Florette Fobasso	Poster

Florette Fobasso (1)

(1) Max Planck Institute for Physics of Complex Systems

We investigated persistent spin polarization in the altermagnet V2Te2O under the addition of spin-orbit coupling. We proposed the realization of collinear persistent altermagnetic spin polarization protected by mirror symmetry in a subclass of 2D altermagnets in the presence of spin-orbit, referred to as persistent altermagnetism. We showed that mirror symmetry protected persistent altermangetism can also emerge in 2D Brillouin Zone sections of 3D altermagnets. Persistent altermagnets are advantageous due to their large nonrelativistic collinear spin splitting, offering promising material realizations for spintronic applications with long spin lifetimes and efficient spin accumulation.

561 **P090**	**Fabrication of Dense Li-Ion–Conducting Li3xLa2/3-xTiO3 Perovskite Ceramics for Electrochemical Devices**	Mikhail Bunevich	Poster

Mikhail Bunevich (1) Ilya Lagutskiy (2) Hryhory Rymski (3)

(1) Belarusian State University of Informatics and Radioelectronics
(2) ATOMTEX SPE
(3) Scientific and Practical Center for Materials Science of the National Academy of Sciences of Belarus

The development of lithium and lithium–air batteries increasingly relies on solid electrolytes and separators with high ionic conductivity. A promising material class for these applications is oxide ceramics based on lithium lanthanum titanate with a perovskite structure. However, practical implementation requires the fabrication of ultrathin, highly dense plates that ensure stable electrochemical performance. In this work, we aimed to identify synthesis and sintering parameters for Li3xLa2/3-xTiO3 ceramics that maximize densification and ionic conductivity.
Polycrystalline Li3xLa2/3-xTiO3 samples were prepared by a citrate–nitrate sol–gel route using titanyl nitrate and lithium and lanthanum salts. To stabilize titanium ions in solution, citric acid was added, followed by ethylene glycol; upon heating, gel formation proceeded via esterification and polymerization reactions. Thermal analysis/heat treatment indicated that crystallization of a single-phase perovskite product occurs in the 950–1000°C range. The primary crystallites formed after this heat treatment were 90–95 nm in size. Elemental composition control by atomic emission spectrometry confirmed that no lithium loss due to volatilization occurs up to 1200°C, which is essential for maintaining stoichiometry. The sol–gel approach provided high powder homogeneity and reactivity, enabling a reduction in the subsequent sintering temperature.
Sintering of pressed compacts at 1200–1300°C yielded ceramic pellets with a relative density of up to 95% of the theoretical (X-ray) density. Microstructural characterization revealed grains with a rectangular cross-section, consistent with tetragonal lattice symmetry. The highest ionic conductivity, measured by electrochemical impedance spectroscopy for samples sintered at 1300°C, reached 1.3 × 10-3 S cm-1. These conductivity values are comparable to those of known analogues and indicate the potential for scaling up the process. As a result, dense pellets with a thickness of 400–600 μm were obtained; due to the combination of high density and ionic conductivity on the order of ~1 mS cm-1, they can be used as separators for lithium–air batteries.

819 **P091**	**Impact of Vanadium Doping on Magnetic Properties and Curie Temperature of HgTe: Heisenberg Model and GGA Study**	Mohamed Baidou	Poster

Mohamed Baidou (1)

(1) Ibn Zohr University, Morocco

The ab initio study was performed using the Generalized Gradient Approximation (GGA) implemented in the CASTEP code to investigate the impact of vanadium doping on the electronic, optical, and magnetic properties of HgTe. The calculated lattice parameters under ambient conditions are in good agreement with the available experimental data. Pristine HgTe exhibits a semimetallic character, where the highest valence-band states slightly overlap with the lowest conduction-band states. Vanadium (V) doping induces ferromagnetism in the system, leading to a high spin polarization of approximately 90% at the Fermi level, making HgTe a promising candidate for spintronic applications. The Curie temperature (TC) was estimated using mean-field theory for doping concentrations of 12% and 24%. The results suggest that the double-exchange mechanism is the dominant interaction responsible for the observed ferromagnetism. Optical calculations also reveal enhanced absorption in the visible and infrared regions, highlighting the potential of V-doped HgTe for optoelectronic applications. These findings provide valuable insights for the development of transition-metal-doped HgTe materials for future spintronic and photonic technologies.

EnS – Energy and Sustainability

EnS – Session 1 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
597	**Supporting Sustainable Heat Pump Deployment through Integrated Planning and Visualization Tools**	Christoph Reichl	Contributed talk (16:00-16:15)

Christoph Reichl (1) Bastian Fibi (1) Michael Wernhart (2) René Rieberer (2) Bernd Windholz (1)

(1) AIT Austrian Institute of Technology GmbH
(2) Graz University of Technology

The large-scale deployment of air-to-water heat pumps is a central component of the transition toward low-carbon heating in residential environments. However, their integration into dense urban settings presents practical challenges that extend beyond energy performance, including spatial constraints, system placement, and community acceptance. Addressing these aspects early in the planning phase is essential to accelerate adoption while ensuring compatibility with existing built environments.
This contribution presents an integrated planning framework that supports decision-making for heat pump installations using a combination of geospatial analysis and immersive visualization. A web-based 2D mapping tool enables the rapid assessment of installation scenarios in real urban contexts, allowing planners to position outdoor units and evaluate their interaction with surrounding structures. This is complemented by a 3D augmented reality environment, which facilitates on-site visualization of planned installations, including system placement, façade integration, and potential mitigation measures.
By linking analytical modeling with intuitive visualization, the approach improves communication between stakeholders, including planners, policymakers, and residents. This enhances transparency in the planning process and helps address acceptance-related barriers, which are increasingly recognized as critical for scaling up heat pump deployment.
The presented framework contributes to more informed and socially robust implementation strategies, supporting the broader goal of sustainable energy system transformation in the building sector.

231	**Advanced Safety Concepts for R290 Heat Pumps in Residential Applications**	Stephan Preisinger	Contributed talk (16:15-16:30)

Stephan Preisinger (1) Felix Hochwallner (2) Heinz Moisi (1) Christoph Reichl (2)

(1) Ochsner Wärmepumpen GmbH
(2) AIT Austrian Institute of Technology GmbH

To replace gas boilers used in multi-family homes safety concepts are crucial for the usage of R290-based heat pumps. While a reduced refrigerant charge mitigates risks, a higher charge allows greater heating capacities, enabling both space heating and domestic hot water production. The FFG-project "WISE" targets a refrigerant charge above 150 g, while ensuring that the maximum releasable charge remains below this limit. Simulations of the charge distribution are used to identify the component holding the largest amount of R290 in the system. Additionally, we evaluate the methods and sensor technologies suitable for detecting possible leakage scenarios. This work summarizes the results of refrigerant simulations and proposes a generic strategy for detecting leaks of indoor R290 heat pumps.

598	**A Database-Driven Approach to Low-Noise Heat Pump Deployment for Sustainable Building Energy Systems**	Christoph Reichl	Contributed talk (16:30-16:45)

Christoph Reichl () Urs Pachale (2) David Goecke (3) Francois Bessac (4)

(1) AIT Austrian Institute of Technology GmbH
(2) Empa
(3) Fraunhofer Institute for Building Physics IBP
(4) CETIAT - Centre Technique des Industries Aérauliques et Thermique

The transition toward air-source heat pumps is a key component of decarbonizing building energy systems. However, noise emissions remain a significant barrier to public acceptance, particularly in dense residential environments. Addressing this challenge requires not only mitigation measures but also improved predictive tools that support optimal system placement early in the planning process.
This contribution presents recent outcomes from the international collaboration IEA HPT Annex 63, which focuses on understanding how installation conditions influence acoustic performance. A central result is the development of an expanded, openly accessible database that compiles detailed acoustic source data for outdoor heat pump units. Unlike conventional metrics based solely on overall sound power levels, the database provides frequency-resolved and direction-dependent information, allowing for more realistic modeling of sound propagation in built environments.
The dataset integrates measurements from multiple laboratories using standardized evaluation and conversion procedures, enabling consistent comparison across different units and test methods. Analysis of representative systems reveals systematic variations in sound radiation depending on unit orientation and component layout, with implications for installation design. For instance, certain unit faces exhibit reduced emission levels, offering potential for passive noise mitigation through strategic placement.
As Annex 63 approaches completion, the work highlights how harmonized acoustic data can support planners, engineers, and policymakers in balancing energy efficiency goals with environmental quality. The results contribute to the development of more reliable prediction models and practical guidelines, facilitating the wider adoption of heat pumps in a socially acceptable and sustainable manner.

743	**III-Nitride Solar Cells: Integrating Advanced Device Physics with Techno-Economic Strategy for Global Energy Transition**	Zine eddine Kaddeche	Contributed talk (16:45-17:00)

Mourad Kaddeche (1) Zine Eddine Kaddeche (2)

(1) Department of Electronics and communication, Faculty of Science and Technology, Djilali Bounaama University of Khemis Miliana, Algeria
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This study presents the design and numerical simulation of high-efficiency p-i-n solar cells based on III-nitride (III-N). By incorporating complex physical models including Fermi-Dirac statistics and Auger and Shockley-Read-Hall (SRH) recombination mechanisms, the work identifies optimal InxGa1-xN/GaN heterojunction configurations to maximize energy conversion efficiency. Beyond technical characterization, the work adopts an interdisciplinary methodology integrating innovation management and cost engineering. The analysis focuses on systematically reducing the cost per peak watt (Wp) through economies of scale and global supply chain optimization. Levelized Cost of Electricity (LCOE) modeling demonstrates that the efficiency gains of InGaN alloys offset higher initial production costs compared to conventional silicon technologies. Ultimately, this study shows that a strong synergy between material innovation and techno-economic planning is the essential driver for the massive and sustainable deployment of third-generation photovoltaics technologies worldwide.

FAKT - Nuclear and Particle Physics

FAKT – Session 1 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
726	**Track Reconstruction with ACTS in Modern High-Energy Physics Experiments**	Alexander J Pfleger	Contributed talk (16:00-16:15)

Gundolf Haase (1) Alexander J Pfleger (1,2) Andreas Salzburger (2)

(1) Uni Graz
(2) CERN

Precise reconstruction of charged-particle trajectories is critical for unlocking the full physics potential of modern high energy physics experiments. Pushing experiments to the intensity and luminosity frontiers results in increasing data rates, bringing existing approaches to their limits. ACTS (A Common Tracking Software) provides a high-performance, experiment-independent toolkit that combines detailed detector geometry, accurate particle propagation in complex magnetic fields, and advanced algorithms for seeding, track finding, and fitting.
The modular design of ACTS enables adaptation to a wide range of detector concepts across high-energy physics, including applications in environments such as the ATLAS at the High-Luminosity LHC and sPhenix at the Relativistic Heavy Ion Collider, as well as detector upgrade and feasibility studies. Ongoing developments position ACTS as an R&D testbed for highly parallelised track reconstruction and the integration of modern ML/AI approaches, driving the evolution of tracking towards robust, portable, and high-throughput solutions for next-generation experiments.

398	**An Intense Antihydrogen Beam for Hyperfine Spectroscopy**	ASACUSA-Cusp Collaboration	Contributed talk (16:15-16:30)

Marcus Bumbar (1) Matti Cerwenka (2) Victoria Kletzl-Teuffenbach (2) Ross Edward Sheldon (2) Martin Simon (2) Eberhard Widmann (2)

(1) University of Vienna (AT)
(2) Marietta Blau Institute, Austrian Academy of Sciences

To date all experiments confirmed invariance of the laws of physics with respect to the combined three discrete symmetries Charge conjugation, Parity, and Time reversal (CPT). Nonetheless, beyond Standard Model physics and the matter-antimatter asymmetry of our universe call for continued searches for CPT violation at the highest possible level of precision. Antihydrogen (Hbar), the bound state of an antiproton and a positron, is the ideal testbench toward this goal as it is a stable atom. Therefore, precise spectroscopy methods with long interaction times are applicable, which are copied from (or can be tested with) hydrogen, the matter counterpart of Hbar. Its hyperfine structure of approx. 1.42 GHz is of particular interest for the most stringent comparisons as it is known to mHz absolute precision.
The ASACUSA-Cusp experiment, based at the Antiproton Decelerator of CERN, aims to measure the ground-state hyperfine structure of Hbar via Rabi-type in-beam spectroscopy. In contrast to existing in-trap results on the Hbar hyperfine structure by the ALPHA collaboration, a beam experiment takes Hbar out of the production traps where high magnetic fields cause challenging systematic uncertainties. This benefit is contrasted by the difficulty of forming a sufficiently intense beam of usable properties, as the beam atoms need to be in the ground state, polarised and within an acceptable velocity range.
Recently, ASACUSA achieved record setting plasma properties and Hbar formation rates, which resulted in an increase in beam intensity by two orders of magnitude of up to 320 Hbar per 15 min. production cycle. The impact of plasma parameters on crucial beam properties like quantum state and velocity distributions can now be studied within reasonable times. We will report on the improvements of the Hbar production, the status of the characterization of Hbar beam properties and potentially the first observation of hyperfine transitions in a beam of Hbar.

270	**GRASIAN: Progress Toward Observing Gravitational Quantum States of Atoms**	Victoria Kletzl-Teuffenbach	Contributed talk (16:30-16:45)

Victoria Kletzl-Teuffenbach (1)

(1) Marietta Blau Institute, Austrian Academy of Sciences

A low-energy particle can be confined by a vertical reflective surface and gravity, settling into so-called gravitational quantum states (GQS). Theoretically predicted for neutrons as well as atoms, only the former have been observed up to now. They were initally detected by Nesvizhevsky et al. and are now routinely used at ILL.
The international GRASIAN collaboration pursues the first observation of GQS of atoms, using a cryogenic hydrogen (H) beam. This is motivated by the availability of higher rates of cold H than what is achievable with current ultracold neutron sources. The resulting higher statistics enable investigations into hypothetical short-range forces between the H and the mirror surface.
This talk will present the current status of the experiment as well as recent measurement results of the first observation of quantum reflection of atomic hydrogen from a silicon mirror surface.

269	**Probing Short Range Interactions with Whispering Gallery States of Neutrons and Hydrogen Atoms**	Katharina Schreiner	Contributed talk (16:45-17:00)

Katharina Schreiner (1,2)

(1) Laboratoire Kastler Brossel
(2) Marietta Blau Institute

Whispering gallery states (WGS) of neutrons and cold atoms, as well as their interferences, are a very powerful tool to probe surface potentials in a curved wave guide. They form in slow particle beams moving along curved surfaces through the effect of the centrifugal force and surface interactions.
Compared to other methods relying on quantum states (such as gravitational quantum states (GQS)), WGS allow us observation of quantum states at higher beam velocities, and they also probe surface interactions at much smaller lengthscales [1,2].
Short range interactions (SRI), mediated by unknown particles between the particle beam and the wave guide, will modify these surface potentials, and leave their imprint on the interferences of the WGS, manifesting as a small observable shift in the interference pattern of several states. WGS measurements are sensitive to SRI at typical lengthscales down to several 10s of nanometers, which is larger than the expected length scale of surface contact interactions, allowing us to eliminate false effects [3].

When placed in a gravitational field, WGS can also be used as a measurement of the gravitational acceleration on the particles in the beam.
We present the current state of preparation of the hydrogen-WGS experiment in Vienna, as well as results of a test measurement using cold neutrons.
Neutrons were used to develop a new measurement and analysis method that allows us to detect small shifts in two-dimensional interference patterns of neutral particles. The measurement method was tested with very small, artificially induced magnetic shifts in polarized neutron beams at the Institut Laue-Langevin (ILL).
Within the GRASIAN collaboration we are currently preparing unprecedented WGS measurements with hydrogen atoms, to be carried out this year, utilizing a cryogenic hydrogen beam with slow horizontal velocities.

[1] Nesvizhevsky, V. et al.: Neutron whispering gallery. Nature Physics, 6, 114--117 (2010). https://doi.org/10.1038/nphys1478
[2] V.V. Nesvizhevsky, A.Yu. Voronin, Centrifugal quantum states of neutrons, Comptes Rendus Physique, 12, p. 791-795 (2011), https://doi.org/10.1016/j.crhy.2011.07.001.
[3] Antoniadis, I. et al.: Short range fundamental forces. Ultra cold neutron quantum states. Comptes Rendus Physique, 12, p.755-778 (2011). https://doi.org/10.1016/j.crhy.2011.05.004}

379	**Low Energy Antiproton Annihilations on Nuclei**	Viktoria Kraxberger	Contributed talk (17:00-17:15)

Viktoria Kraxberger (1)

(1) Austrian Academy of Sciences (AT)

Antiproton–nucleus annihilation at rest is a complex process that is not yet fully described by existing models, particularly due to the scarcity of experimental data on production of heavy nuclear fragments, which has led to a limited understanding of final state interactions (FSI). New measurements are therefore essential to validate models of the annihilation dynamics and to clarify how the primary mesons interact with the nuclear medium.
In this work, antiproton annihilations at rest in thin solid targets are studied at the AEgIS facility at CERN. The multiplicity, energy, and angular distributions of the emitted particles are measured using a system of Timepix4 detectors, providing access to the characteristics of the annihilation products and their evolution with the nuclear mass. These observables enable a systematic investigation of FSI effects and their impact on particle production and yields.
A reconstruction algorithm has been developed to determine the three-dimensional annihilation vertex from particle tracks in single-plane detectors. In contrast to conventional multi-layer tracking approaches in high-energy physics, this method achieves vertex reconstruction using a single detection layer, allowing a clean selection of annihilation events in the target. Preliminary results will be presented and discussed.

332	**Status and Recent Developments of the NUCLEUS Experiment**	Lorenzo Valla	Contributed talk (17:15-17:30)

Lorenzo Valla (1)

(1) Austrian Academy of Sciences (AT)

Coherent elastic neutrino-nucleus scattering (CEvNS) is a weak neutral-current process predicted by the Standard Model of Particle Physics. A neutrino scatters elastically and coherently off a nucleus, yielding a low-energy nuclear recoil in the eV-keV range. Such a low-energy signature makes the detection of the process extremely challenging.
The NUCLEUS experiment, located at the Chooz nuclear power plant, aims to study CEvNS on tungsten nuclei using neutrinos produced by the two 4.25 GWth reactor cores. To do so, NUCLEUS deploys gram-scale CaWO4 crystals, operated as cryogenic calorimeters with an ultra-low nuclear recoil energy threshold of O(10) eV. The crystals are instrumented with Transition Edge Sensors, operated at ~10 mK, to read out the phonon signal directly. The shallow overburden provided by the site also requires an elaborate system of active vetoes and passive shielding to mitigate the backgrounds.
After a commissioning phase, the experiment is starting to collect data in a year-long technical run, to assess noise and background conditions in-situ, as well as to set first limits on the CEvNS cross section on tungsten and constrain beyond-the-Standard-Model interactions. In the talk, I will present an update on the latest developments of NUCLEUS.

FAKT – Session 2 (Wed 23, 10:30-12:30)

ID	Title	Speaker	Type
722	**Searches for Long-Lived Particles at the Upsilon(4S)**	Abi Soffer	Contributed talk (10:30-10:45)

Abi Soffer (1)

(1) Tel Aviv University (IL)

Electron-positron colliders at the Upsilon(4S) resonance are capable not only of flavor-physics studies, but can also search for new particles beyond the standard model. I will describe such proposed searches, focusing on the case of long-lived particles.

643	**Glueballs and Mesons from Functional Equations**	Markus Huber	Contributed talk (10:45-11:00)

Markus Huber (1)

(1) Giessen University

QCD has a rich spectrum that encompasses bound states of different types. In pure Yang–Mills theory the spectrum consists of glueballs, which are also expected to be realized in the presence of quarks. The former theory provides a clean theoretical setup in which the spectrum has been established by various methods, including functional equations. In a top-down approach, these equations provide a framework that does not require external model input. To progress toward full QCD, the existing solutions for gluonic correlation functions are used as a basis for including quarks. Particular attention is paid to constructing a truncation that respects chiral symmetry so that it can be applied to light mesons.

446	**Quantum Simulation of Generalized Parton Distributions: A Qudit-Based Approach**	Florian Hechenberger	Contributed talk (11:00-11:15)

Florian Hechenberger (1) Tommaso Rainaldi (1) Felix Ringer (1) Ismail Zahed (1)

(1) Stony Brook University

With the future Electron Ion Collider on the horizon, Generalized Parton Distributions (GPDs) have attracted significant interest over the past years. As a tool to map out the three-dimensional structure of hadrons, they offer unique opportunities to study Quantum Chromodynamics (QCD) and complex partonic correlators at non-perturbative scales. However, their experimental extraction is complicated by the deconvolution problem, model dependence, and the limited reach of current lattice calculations. Quantum computers, including qudit-based architectures, offer a potential route to study such observables in a controlled setting.
In this talk, I present an 8-dimensional qudit formulation of the $SU(3)$ color structure of QCD_{1+1} on a lattice. After introducing the baryon and boost operators, I show how the off-forward matrix elements relevant for GPDs can be measured directly on quantum hardware, avoiding an explicit deconvolution step in this framework. I validate the approach using state-of-the-art tensor network simulations, estimate the resource requirements, and feasibility of the required measurements on current and near-term quantum devices.

470	**Hadron Structure from Contour Deformations**	Eduardo Ferreira	Contributed talk (11:15-11:30)

Eduardo Ferreira

The internal structure of hadrons can be described in terms of structure functions that encode, for example, the momentum and spin distributions of their constituents. Parton distribution functions (PDFs) and Transverse Momentum Distributions (TMDs), for example, describe the quark and gluon momentum distributions inside a hadron. These distribution functions are, however, not easy to calculate, because they are defined on the light front, whereas most hadron calculations are performed in a Euclidean metric.
In this talk, we are present a new method we are developing to compute these parton distributions from hadronic matrix elements using contour deformations. We will illustrate the method for a simple system of two interacting scalar particles of equal mass. This calculation includes both self-consistent inputs: the Bethe-Salpeter amplitude (calculated from its Bethe-Salpeter Equation), and the four body scattering matrix (to access beyond valence contributions). We will also explore the steps needed for application to first principles QCD.

314	**$\Lambda_c(2595)$ at Belle II: Extending Event Generation with Herwig**	Cristhian Xavier Brito Ricaurte	Contributed talk (11:30-11:45)

Cristhian Xavier Brito Ricaurte (1) Christoph Schwanda (1)

(1) Austrian Academy of Sciences (AT)

The Belle II detector is a general-purpose spectrometer built around the interaction point of the asymmetric-energy electron–positron collider SuperKEKB, located in Tsukuba, Japan. While Belle II is best known as a B-factory, the production rate of charm–anticharm quark pairs at SuperKEKB is slightly higher than that of B-meson pairs. To date, charm and light quark hadronization at Belle II has been simulated using PYTHIA 8. However, the implementation of Pythia at Belle II does not account for excited charm baryons. As a result, the development of alternative strategies for studying these baryons has become increasingly important. In this contribution, I discuss the role of the $\Lambda_c(2595)$ as an entry point for improving our understanding of the excited spectrum of charm baryons, and I share some preliminary results on the characterization of this orbitally excited state at Belle II using a newly implemented Monte Carlo generator: Herwig.

444	**Higher-Spin Baryons with Functional Methods**	Luca Oberguggenberger	Contributed talk (11:45-12:00)

Luca Oberguggenberger (1)

(1) University of Graz

In a relativistic quantum field theory like Quantum Chromodynamics (QCD), there is no upper bound on the spin of a hadron. Baryon resonances have been experimentally confirmed for the Nucleon and Δ baryons up to spin $J^P = 15/2^+$ range with varying certainty. Of the higher-spin baryons, generally meaning baryons with J > 3/2, only a select few have been treated using functional methods such as Bethe-Salpeter equations (BSE) – in part, because these calculations quickly escalate in complexity in the three-body picture of the baryon. The diquark picture, which views baryons as quark-diquark bound states, on the other hand, provides an interesting venue to study higher-spin resonances, where most of these complications are absent. In this approach the bound-state equation for the diquark takes, apart from its color structure, the same shape as the meson BSE. The resulting diquark Bethe-Salpeter-amplitude is combined with the remaining quark and diquark ingredients in a rainbow-ladder truncation into a quark-diquark BSE, which is solved by converting it to an eigenvalue problem.
The corresponding spectrum of light, spin J = 1/2 and 3/2 baryons has been extensively studied in the past. As an extension of these considerations, this talk focuses on the expansion of the light quark-diquark baryon spectrum into the higher-spin regime.

FAKT – Session 3 (Thu 24, 10:30-12:30)			
ID	Title	Speaker	Type
354	**What is Negative Coupling Field Theory?**	Paul Romatschke	Contributed talk (10:30-10:45)

Paul Romatschke (1)

(1) TU Wien

Quantum Field Theory is a mature technology that is highly predictive. Most textbooks construct quantum field theory as an expansion for small positive coupling around classically stable vacua, which is a perfectly reasonable thing to do. However, history tells us that quantum mechanics sometimes does not conform to classical intuition. For instance, the hydrogen atom does not have a classically stable ground state, but is stable quantum mechanically. Similarly, negative coupling systems typically have upside-down potentials that do not possess a classically stable ground state. In this talk, I will give arguments why some negative coupling systems nevertheless are stable and physically acceptable quantum mechanically. In these theories, physical observables behave reasonably, with no indication of instabilities despite the missing classical intuition. I will point out the curious implications for our understanding of quantum field theory as well as for high energy physics observables that arise from treating negative coupling field theories as acceptable continuum descriptions of nature.

381	**The FMS Mechanism as a Tool for Semiclassical Calculations in Quantum Gauge Theories**	Axel Torsten Maas	Contributed talk (10:45-11:00)

Axel Torsten Maas (1)

(1) University of Graz

In many gauge theories the dynamics is dominated by a classical solution with small fluctuations around it. The primary examples are electroweak physics and quantum gravity, but also many proposed extensions of the standard model like grand-unified theories.
The Fröhlich-Morchio-Strocchi (FMS) mechanism is a manifestly gauge-invariant approach augmenting perturbation theory to describe matrix elements in these settings, and has been demonstrated to be superior to perturbation theory alone. This mechanism is outlined and some pertinent examples are given, especially in cases where ordinary perturbation theory does not prove fully satisfactory results.

392	**Temporal and Spatial Structures in the Sauter-Schwinger Effect**	Matthias Diez	Contributed talk (11:00-11:15)

Matthias Diez (1) Reinhard Alkofer (1) Christian Kohlfürst (2)

(1) Universität Graz
(2) Helmholtz-Zentrum Dresden-Rossendorf

Pair creation in extremely strong electric background fields— the Sauter–Schwinger effect—has long been predicted theoretically. However the time and length scales over which particles are formed, has remained difficult to determine.
In this work, we investigate these temporal and spatial scales by analysing the time evolution of physical observables in spatially and temporally structured electric fields using the Dirac–Heisenberg–Wigner formalism.
To interpret the behaviour of these observables at intermediate times, we introduce a hypothetical procedure in which the external field is switched off at a given instant in time.[1] This approach enables us to examine particle and charge densities at pre-asymptotic times.
Based on this method, we identify distinct time scales in both position and momentum space. Furthermore, we carry out a systematic parameter study and extract power-law dependencies of these time scales for pair production driven by a single Sauter pulse [2] and show that in the case of the dynamically assisted Schwinger effect, the pair production process seems to happen in a significantly shorter time [3].

[1] A. Ilderton, Phys. Rev. D 105, 016021 (2022)
[2] M.Diez, R.Alkofer, C.Kohlfürst, Phys. Lett. B 844, 138063 (2023)
[3] M.Diez, R.Alkofer, C.Kohlfürst, „Temporal and Spatial Scales in Particle production from Ultra-Strong Fields", in preparation

256	**Kernels and Cycles in Real Time Complex Langevin**	Enno Carstensen	Contributed talk (11:15-11:30)

Enno Carstensen (1) Dénes Sexty (1)

(1) University of Graz

Real time evolution in QFT poses a severe sign problem, which may be alleviated via a complex Langevin approach. However, simulation with large real-time extent give incorrect results. A kernel in a complex Langevin equation is known to influence the appearance of the boundary terms and integration cycles, and thus kernel choice can improve the range of real-time extents with correct results. For multi-dimensional models the optimal kernel is searched for using machine learning methods. We test this approach by simulating the simplest possible case, a 0+1-dimensional scalar field theory in Minkowski space.

311	**The Analytic Structure of the Quark Propagator for Timelike Momenta**	Felix Halbwedl	Contributed talk (11:30-11:45)

Felix Halbwedl (1)

(1) University of Graz

The quark propagator is one of the basic building blocks required to compute physical properties of hadronic bound states via Bethe-Salpeter equations. While it is a routine task nowadays to calculate it nonperturbatively for a wide range of real spacelike momenta via the Quark Dyson-Schwinger Equation (DSE), its direct computation for generic complex momenta remains challenging and depends on the Vertex Ansatz needed as an input for the DSE.
The aim of this work is to compare and complement commonly employed extrapolation methods with more recently used complex domain methods like the Cauchy or contour deformation ones to examine the quark propagators analytic structure for different Vertex Ansätze (Rainbow Ladder, Ball-Chiu).

695	**Infrared Quark–Gluon Vertex and Pion Structure in Minkowski Space**	Vinícius Raimundo	Contributed talk (11:45-12:00)

Vinícius Raimundo (1) Murilo Pedroso (1) Wayne de Paula (1) Tobias Trederico (1)

(1) ITA - Instituto Tecnológico de Aeronáutica

In this work, the pion is described by the Bethe–Salpeter wave function (BSWF), obtained by solving the corresponding bound-state equation formulated in Minkowski space. Established results from lattice QCD calculations for light quarks and gluons are employed to model the kernel of the Bethe–Salpeter equation (BSE) and to dress its constituents. In addition, we implemented a dressed quark–gluon vertex via an ansatz that incorporates a nontrivial infrared (IR) structure in the BSE, which is solved in Minkowski space using an integral representation. Within the adopted model, we explore the impact of the IR behaviour of the quark–gluon vertex on the internal structure of the pion by computing the valence wave function, which is obtained by projecting the BSWF onto the light front. The associated unpolarized parton distribution function and other related observables are calculated. These quantities are of current interest and will be further investigated in future electron–ion colliders.

FAKT – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
308 **P092**	**Far Field Measurements of Gravitational Quantum States of Cold Atomic Hydrogen**	Melanie Federer	Poster

Melanie Federer (1)

(1) Marietta-Blau Institut, ÖAW

At very low transversal energies, light neutral particles above a horizontal reflective surface can undergo quantum reflection forming gravitational quantum states (GQS). While these states have been experimentally observed only for neutrons in 2002 by V.V. Nesvizhevsky et al., theory predicts their existence also for atoms. GQS provide a sensitive probe for new fundamental short-range interactions predicted in extensions of the Standard Model and in models explaining dark matter and dark energy [1;2].
In the far field, interference of quantum states emerges, providing a powerful tool for high-sensitivity measurements. Small shifts in the interference pattern can arise from external interactions. While gravity induces a mass-dependent shift, unknown interactions would produce additional deviations. In contrast to GQS transmission measurements, which primarily confirm the existence of such states, far field interference measurements enable substantially higher precision and allow surface-dependent short-range interactions to be probed and constrained [3].
We present the current state of preparation for far field measurements of GQS of atomic hydrogen in Vienna. The experiment utilizes a cryogenic beam with low horizontal velocities. To measure the GQS, a one-component gravitational spectrometer is used. This spectrometer consists of a flat mirror on the bottom and a macroscopically flat scatterer on top separated by a gap of variable size . The preparations for the first measurements of GQS with atomic hydrogen and for the far field measurements are ongoing.

[1] C. Killian et al. GRASIAN: towards the first demonstration of gravitational quantum
states of atoms with a cryogenic hydrogen beam. The European Physical Journal D, (3), 2023. doi: 10.1140/epjd/s10053-023-00634-4.
[2] V. V. Nesvizhevsky et al. Quantum states of neutrons in the earth's gravitational field. Nature, 2002. doi: 10.1038/415297a.
[3] V. V. Nesvizhevsky et al. Gravitational and other shifts of whispering gallery and gravitational state interference patterns of light neutral particles, 2025.

493 **P093**	**Free Neutron Decay with PERC - A status Update**	Johannes Maximilian Schilberg	Poster

Johannes Maximilian Schilberg (1) Hartmut Abele (1) Erwin Jericha (1)

(1) Atominstitut - TU Wien

The PERC (Proton and Electron Radiation Channel) facility, located at the neutron source FRM II of the Technical University of Munich (TUM), serves as a clean source of neutron decay products (protons and electrons). PERC aims to contribute to the determination of the Cabibbo-Kobayashi-Maskawa quark-mixing element (V_ud), measure the correlation coefficients of free neutron decay (a, A, b, C) and search for new physics at the TeV scale. For this, all systematic errors will be controlled beyond 10^(-4) level. In order to achieve this, the PERC detector system will consist of a primary detector and two backscattering detectors to detect the 2% of electrons that are backscattered from the main detector. To ensure a low background for the detectors as well as to fulfil all radiation protection requirements, the PERC beamstop has been designed. Its components will consist of boron carbide (B4C) and lead (Pb), which were chosen based on MCNP simulations.

438 **P094**	**Chiral Restoration and Deconfinement in Finite-Temperature Quenched *SU(3)***	Alireza Sharifian	Poster

Alireza Sharifian (1) Leonid Glozman (1) Denes Sexty (1)

(1) University of Graz

A fundamental question in finite-temperature QCD is the relation between chiral symmetry restoration and deconfinement. In real-world QCD these phenomena are usually seen as a common crossover, while theoretical arguments suggest that in the large-N_c limit they may become distinct phase transitions, possibly separated by an intermediate confining but chirally symmetric phase. As a first step toward addressing this problem, we study finite-temperature quenched $SU(3)$ gauge theory on the lattice. We analyze the temperature dependence of the low-lying spectral density of the overlap Dirac operator, which is directly related to the chiral condensate through the Banks-Casher relation, together with the Polyakov loop as an indicator of deconfinement. This study provides the first step toward a systematic extension to higher N_c and toward clarifying the possible existence of an intermediate phase.

GEP - History of Physics

M06 – Session 1 (Mon 21, 16:00-18:00, Chair: Bruno Besser)			
ID	Title	Speaker	Type
52	**A Brief History of Victor Weisskopf, a Unique 20th Century Physicist**	Walter Kutschera	Invited talk (16:00-17:00)

Walter Kutschera (1) Peter Illetschko (2)

(1) University of Vienna, Faculty of Physics
(2) Independent Science Journalist, Vienna

Victor Weisskopf (1908-2002) belonged to the generation of 20th century physicists who experienced the development of quantum physics in the 1920s and 1930s as well as the Manhattan project and the rise of accelerator-based physics after the Second World War.
He was a theoretical physicist at heart, but like other great physicists of his generation (e.g. Enrico Fermi) he knew "everything" in physics. In 1991, Weisskopf described his extraordinary life in a beautiful autobiography [1]. He visited his hometown Vienna for the last time in 2000, when a symposium in memory of the 100th birthday of Wolfgang Pauli was held at the University of Vienna. Very recently, a new biography on the life of Victor Weisskopf was published in German, which describes his life between science and conscience [2]. In this contribution, an effort will be made to describe the many facets of the life of Victor Weisskopf in a concise form.

[1] V. Weiskopf, 1991. The Joy of Insight – Passions of a Physicist, Basic Books, New York
[2] P. Illetschko, 2026. Im Schatten der Atombombe: Victor Weisskopf – ein Physikerleben zwischen Wissenschaft und Gewissen, Residenzverlag Salzburg-Wien.

640	**Astronomical Use of Camera Obscura to Monitor Solar Eclipses before Telescope's Area**	Mohammed Boudjada	Contributed talk (17:00-17:20)

Mohammed BOUDJADA (1) Bruno Besser (1)

(1) Space Research Institute, Austrian Academy of Sciences, Graz, Austria

It is well-known that Kepler (1571-1630) provided optical principle of the telescope, the astronomical lunette, to Galileo (1564-1642), who used it to discover and investigate physical aspects of the Moon, and Jupiter's satellites. Kepler's knowledge was not restricted to the telescope (i.e., lens, objective and ocular) but included also the optics known since Greeks. In this study, we attempt to examine the instrumental role of the camera obscura, or pinhole, at the end of sixteenth century and the beginning of the seventeenth one. This time interval marks the emergence of the heliocentric system mainly due to the high accuracy of the observations, and the 'mathematization' of the instrument concepts, as well the separation from astrology and astronomy. Hence, the camera obscura was used for Solar eclipse observations despite the complexity of the measurement interpretations. Kepler attempted in Graz to plan the observation of the Solar eclipse of 10 July 1600, never detailed the outcomes but reported about other eclipses. Through this work, we emphasize on the progressive evolution of the camera obscura as an astronomical instrument, and discuss Kepler's approaches to solve the optical difficulties faced during the Solar eclipses.

707	**The Mystery of Boltzmann's Bizykel**	Heinz Krenn	Contributed talk (17:20-17:40)

Heinz Krenn (1)

(1) Institute of Physics, University of Graz

Even before his 1890 appointment at LMU Munich, Ludwig Boltzmann had ordered his mechanical engineer in Graz, Anton von Gasteiger, to build a mechanical model that was then further developed in Munich 1890 as the "Bizykel"—an "inexplicable apparatus with a gear mechanism". Both the Graz and Munich original models were lost, so that only replicas exist in historical museums today. Following the undoubted success of Maxwell's theory of electromagnetism, Boltzmann turned his attention to illustrating the analogy between cyclic (periodic) electromagnetic phenomena and simple mechanical constructions. It served as a didactic approach [1] to visualizing electromagnetic phenomena such as Faraday's law of self-induction and the transport of energy in lumped electrical circuits. Today, the path to understanding electromagnetic circuits has been reversed: Physicists are more familiar with electric networks (since they are easier to construct). Boltzmann's bicycle demonstrates how a two-coil arrangement (known as an electric transformer) can be simulated as a "Zahnradgetriebe mit 3 Konusrädern". To the best of the author's knowledge, and despite a wealth of descriptive articles on Boltzmann's bicycle [2] and Paul Ehrenfest's obituary for Ludwig Boltzmann [3], a comprehensive explanation of the bicycle's principle from a modern perspective is missing. This will be addressed here using the example of an open and short-circuited electric transformer.

[1] L. Boltzmann: Vorlesungen über Maxwell's Theorie der Elektricität und des Lichts, 1. Theil, Leipzig: Johann Ambrosius Barth 1891
[2] H. Ebert: Mechanisches Modell zur Erläuterung der Inductionsgesetze = Bizykelmodell, Annalen der Physik und Chemie, Bd. XLIX, Leipzig: Johann Ambrosius Barth 1893, 642-650.
[3] P. Ehrenfest: Ludwig Boltzmann's mechanische Deutungen, Necrology, Mathematisch-Naturwissenschaftliche Blätter 1906, No. 12.

710	**Peter Apian - A Pioneer in Astronomical Instrumentation**	Sonja Draxler	Contributed talk (17:40-18:00)

Sonja Draxler (1)

(1) Institute of Physics, University of Graz

Peter Apian was a German humanist, known for his works in mathematics, astronomy and cartography. His books were extremely influential in his time, with the numerous editions in multiple languages being published until 1609.One of the most important astronomical discoveries of Apian resulted from his observations of comets. Apian realized that the comet's tail always points away from the sun, and he was the first to publish drawings of the direction of the comet's tail. Apian's most important work is the Astronomicum Caesareum from 1540, which he dedicated to Emperor Charles V and his brother King Ferdinand I. Its special feature is the 36 full-page woodcuts, 21 of which are provided with rotating paper discs, so-called volvelles. They reproduce the Ptolemaic system and serve as calculating discs that make it possible to determine the position of the planets.

LHS – Physics and School

LHS – Session 1 (Tue 22, 16:00-18:00, Chairs: Alexander Strahl and Susanne Neumann)			
ID	Title	Speaker	Type
808	Preisträgervorträge der VWA-Preisträgerinnen und -Preisträger der ÖPG 2026	VWA-PreisträgerInnen	Contributed talk (5 x 10 min.)
809	Vorstellung des IYPT Tournament	IYPT-TEAM	Contributed talk (15 min.)
810	Vorstellung der Physikolympiade	PO-Team	Contributed talk (15 min.)

MBU - Physics in Medicine, Biology and Environment

MBU – Session 1 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
505	**Predicting Allostery, the "Second Secret of Life"**	Sandro Keller	Contributed talk (16:00-16:15)

Sandro Keller (1) Moritz Smilde (1) Varvara Vetrova (1)

(1) University of Graz

Allostery—the functional coupling between distant sites in a protein—underlies biological regulation from signal transduction to metabolism and is a major target in drug discovery. The idea that allostery arises from shifts in a protein's conformational ensemble has gained broad acceptance over the past decades, but these conceptual advances have not been turned into quantitative, predictive tools.
We address this challenge for the case of two ligands binding to the same protein, where allosteric cooperativity can be captured by a single thermodynamic parameter. To this end, we sample conformational ensembles of proteins in different ligation states using atomistic molecular dynamics (MD) simulations, quantify probability densities in conformational space, and extract the cooperativity parameter through information-theoretic inference. The approach is model-free and general, works with equilibrium MD trajectories, and requires neither enhanced sampling nor predefined reaction coordinates.
I will present the underlying statistical-mechanical framework, its computational implementation, and its validation against experimentally well-characterized allosteric proteins. Beyond these specific systems, simulation-based prediction may open new avenues for understanding and exploiting allostery in drug design.

458	**Large-Volume Plasma Focused Ion Beam Tomography of Mast Cells: Workflow, Optimization, and Applications**	Heiko Groiss	Contributed talk (16:15-16:30)

Heiko Groiss (1) Alexey Minenkov (1) Sara Hirner (1) Lena Wiesbauer (1) Philip Steiner (1)

(1) Johannes-Kepler-Universität Linz

We present a practical, high-quality workflow for large-volume plasma focused ion beam-scanning electron microscopy (PFIB-SEM) tomography on mast cells. Beyond their classic roles in allergy, mast cells are vital for tissue homeostasis, repair, and defence, yet aspects of their ontogeny and functions in cancer and cardiovascular health remain unresolved. Progress requires ultrastructural reconstructions and segmentation of the numerous vesicles and granules, a step that is still largely carried out manually. Given that robust AI model training demands extensive datasets, we employed large-volume Xenon PFIB-SEM tomography, to accelerate data acquisition and extend an established correlative light and electron microscopy (CLEM) workflow with AI based segmentation.
A key challenge in PFIB-SEM of high-pressure frozen, cryo-substituted mast cells embedded in epoxy is mitigating charging and thermal damage while preserving a smooth, artefact-minimized surface. We addressed this by adding conductive carbon nanoparticles to the resin; a 5% loading best suppressed charging while maintaining workable viscosity. Following optimization of the slicing conditions at 30 keV, combined with stage rocking, we achieved smooth sections with minimal curtaining. For SEM imaging at 5 keV, a low-energy backscattered electron detector delivered the highest signal-to-noise ratio and enhanced ultrastructural contrast. Using these settings, it is possible to generate both large datasets comprising several cells with a voxel size of 50 nm and high-resolution reconstructions with ca. 1000 slices and isotropic voxels of 7 nm.
We will detail the workflow and initial AI-segmentation results and discuss how PFIB-SEM accelerates the collection of large, high-fidelity datasets, thereby representing a promising method for further pathology-relevant cells and tissues.

464	**AI-Based Gait Analysis as a Dynamical System: Integrating Stability, Variability, and Expression in Human Movement**	Peter Hüttner	Contributed talk (16:30-16:45)

Peter Hüttner (1) Ille C. Gebeshuber (1) Richard W. van Nieuwenhoven (1)

(1) TU Wien, Institut für Angewandte Physik

This study presents a data-driven framework for analysing human gait as a dynamical system using multimodal sensor data. The approach combines high-resolution plantar pressure measurements—i.e., the spatial distribution of contact pressure between the foot and the ground—obtained from instrumented insoles, with time-synchronised physiological signals and contextual annotations across multiple repeated measurements in real-world conditions.
Data acquisition was performed using wearable pressure sensors capturing spatio-temporal load distribution across 16 channels (8 per foot), enabling reconstruction of step sequences, load transfer patterns, and centre-of-pressure dynamics. Measurements were conducted under varying conditions, including baseline walking, externally influenced contexts (e.g. footwear changes and environmental conditions), and repeated trials per subject, resulting in a dataset with high intra-individual variability.
The analysis pipeline comprises:
1. preprocessing and temporal alignment of sensor streams,
2. extraction of gait features (step timing, pressure integrals, spatial distribution),
3. computation of variability metrics (intra-step and inter-step variance), and
4. evaluation of condition-dependent changes across repeated measurements.
Results indicate that gait patterns exhibit structured variability rather than random noise. Across repeated trials, individuals demonstrate consistent baseline signatures, whilst condition changes induce reproducible shifts in pressure distribution, step dynamics, and variability measures. Both increases and decreases in variability were observed depending on the type of perturbation, suggesting that variability is context-dependent rather than unidirectional.
These findings support the interpretation of gait as a dynamically stable system operating within a bounded region of variability, where deviations reflect adaptive responses to internal and external constraints rather than necessarily pathological states.

631	**Metabarcoding as a Key Tool to Demonstrate Natural Attenuation of HTF via Denitrification**	Norbert Nägele	Contributed talk (16:45-17:00)

Cynthia Alcántara (1) Norbert Nägele (1) Jorge Diamantino-Miranda (1)

(1) Kepler, Ingenieria y Ecogestion, S.L.

Sampling campaigns are performed periodically by KEPLER at a site contaminated with heat transfer fluid (HTF), a thermal oil used in solar thermal plants. The results obtained showed that when the concentration of HTF decreased in piezometers nitrites (NO2-) production was detected in groundwater. This fact suggested a possible removal of HTF via biological denitrification of the pollutant where nitrate is used as an electron acceptor under anoxic conditions. The denitrification metabolic pathway consists of the reduction of nitrates (NO3-) to nitrogen gas. This process occurs in successive stages, catalyzed by different enzymatic systems, with nitrites (NO2-), nitric oxide (NO) and nitrous oxide (N2O) appearing as intermediate products. Thus, if HTF could be being used as a source of organic carbon during a denitrification process, an active natural attenuation process could be demonstrated in the aquifer.
To study this hypothesis, KEPLER carried out a metagenomics study in which the genomic region of the 16S ribosomal gene was analyzed to identify the autochthonous population of the aquifer and thus verify if there were denitrifying microorganisms. From the 16S sequences identified, a functional analysis was also carried out to infer the metabolic functions that could take place in the aquifer and check if denitrifying enzymes were present. After the metagenomics analysis, a laboratory treatability study was also carried out to evaluate a possible removal of HTF in the aquifer groundwater by this biological denitrification pathway. For that, a continuous test was performed in which a reactor under anoxic conditions was fed with HTF and nitrate for 6 months to evaluate the potential of the natural attenuation process.
Metagenomics study demonstrated that among the most abundant genera in the autochthonous microbial community were some that participate in denitrification processes using nitrate as an electron acceptor under anoxic conditions, such as the genus Thauera spp. The ability of this genus to degrade aromatic compounds, as are HTF and its by-products, was also observed in denitrification reactors. Other microorganisms that play an important role in the nitrogen cycle were also identified, such as the genera Nitrosomonas spp. and Nitrospira spp. and, within the archaea group, the genus Nitrosarchaeum spp. Among the potential metabolic functions, enzymes described as denitrifying agents were identified such as nitrate reductase, nitrite reductase, nitric oxide reductase and nitrous oxide reductase. The presence of these microorganisms and these enzymes indicates that denitrification may occur in the aquifer and, furthermore, reinforces the hypothesis that HTF can be degraded by denitrification in an anoxic environment.
Treatability study in a continuous reactor confirmed the presence of a denitrification metabolic pathway. In this test it was observed that when HTF or NO3- were added separately, the concentrations of these two compounds did not decrease, however, when adding them simultaneously, HTF consumption and transformation of NO3- into NO2-, confirming that HTF can be removed from groundwater via biological denitrification.
In conclusion, this study provides the first evidence of the effectiveness of denitrification to eliminate HTF during groundwater treatment and highlights the potential of using genetic tools in the evaluation of soil and groundwater natural attenuation. In this case study, the demonstration of natural biodegradation of HTF to local authorities made it possible the application of a groundwater control and monitoring program and discard an active remediation strategy in the aquifer.

MBU – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
114 **P036**	**Computational Mechanistic Study of Anticancer Drug Encapsulation in Nanotubes**	Mansoor Alshehri	Poster

Mansoor Alshehri (1)

(1) Department of Mathematics, College of science, King Saud University, Riyadh, Saudi Arabia

Cancer remains a leading cause of morbidity and mortality worldwide. Chemotherapy with antitumor drugs is the most common treatment, but its effectiveness is often limited by toxicity and damage to healthy cells. Nanotubes, owing to their unique geometric and mechanical properties, have emerged as promising nanocarriers for targeted drug delivery. In this study, we employed a continuum modeling approach with the 6–12 Lennard–Jones potential to investigate the encapsulation of 5-Fluorouracil (5-FU), a widely used anticancer drug, in single-walled carbon, silicon, and boron nitride nanotubes. Interaction energies and equilibrium positions were computed to determine the most suitable nanotube type and size for efficient drug encapsulation. Our results indicate that the optimal radii for 5-FU encapsulation are approximately 6.08 Å, 5.98 Å, and 6.05 Å for carbon, silicon, and boron nitride nanotubes, respectively. The corresponding interaction energies of −16.55, −17.81, and −18.20 kcal/mol suggest favorable drug-nanotube interactions across all three materials. These findings provide insights into the design of nanotube-based drug delivery systems, highlighting how the choice of nanotube material and size can influence drug loading efficiency. This study demonstrates the potential of computational approaches to guide the development of more effective and selective anticancer therapies.

162 **P037**	**Computation of a Consistent System Matrix for Cone-Beam Computed Tomography**	Josef Simbrunner	Poster

Josef Simbrunner (1) Andreas Habring (2) Clemens Krenn (2)

(1) Medical University Graz
(2) Institute of Visual Computing, Graz Technical University

One of the main challenges in algebraic reconstruction techniques (ART) for computed tomography (CT) is the generation of the matrix of the weighting coefficients, also called system matrix (SM). It is well established that in theory the exact SM entries are computed as the relative sub-voxel volumes covered by X-rays towards a detector element. However, due to high computational efforts, in practice approximations based on line integrals are frequently used. In this work, we propose a novel method for the computation of the exact system matrix for two- and three-dimensional cone-beam flat-detector CT. The method relies on the decomposition of the cone-voxel intersection volumes into subvolumes that contribute to distinct detector elements and whose contributions to the system matrix admit analytical expressions that can be evaluated without costly iterative subroutines. We demonstrate that the reconstructions obtained with the proposed method are superior to those obtained with common line-based integration approaches with numerical experiments on synthetic CT data.

175 **P038**	**Traction Force Microscopy for Probing Mechanical Signatures of Breast Cancer Progression**	Jose L. Toca-Herrera	Poster

Jose L. Toca-Herrera (1) Juan Carlos Gil-Redondo (1,2) Andreas Weber (13) Maria dM Vivanco (4)

(1) BOKU Univesrity, Austria
(2) CBM-CSIC, Spain
(3) UCL, UK
(4) CIC BioGUNE, Spain

Cells generate traction forces to probe the mechanical properties of their surroundings and to maintain a basal equilibrium state of stress. These forces also play key roles in cell migration, adhesion, and extracellular matrix (ECM) remodeling, and their dysregulation is frequently associated with pathological conditions such as cancer. Quantifying traction forces is therefore essential for understanding cell mechanics in cancer progression and metastasis.
In this work, we present a practical primer on two dimensional traction force microscopy (2D TFM), outlining the experimental workflow and data analysis methodology. As an application example, we measured traction forces generated by three human breast cancer cell lines with distinct metastatic potential (MCF10-A, MCF-7, and MDA MB 231) and examined how disruption of the actin cytoskeleton affects these forces. Contrary to common assumptions in the literature, we observed that cells with higher metastatic potential (MDA MB 231) exerted lower traction forces. We discuss how substrate stiffness and ECM protein concentration may contribute to these findings and influence the interpretation of traction force measurements in cancer research.

268 **P039**	**The Role of Carotenoid-Protein Interactions for the Colour Change of Grasshopper Wings**	Eva Pichler	Poster

Eva Pichler (1) Limin Wang (1) Bodo Wilts (1)

(1) University of Salzburg

Colour changes in animals serve various functions, such as communication, camouflage, and thermoregulation [1]. In insects, coloration arises from structural colours and pigments. While structural colours result from light interference, pigment-based colours originate from selective light absorption and reflection of unabsorbed light. Some organisms exhibit colour-changes as a response to external stimuli such as temperature, humidity, and pH differences [2]. Recent studies have shown that the wings of the grasshopper Coloracris azureus exhibit a reversible thermochromic shift from blue to red when heated from 30 °C to 100 °C (i.e. outside the physiological range) [3]. These colour changes arise from the reversible binding and unbinding of the carotenoid astaxanthin to a protein, which is thought to be responsible for the observed thermochromic behaviour
The present project aims to further investigate the carotenoid–protein interactions responsible for this phenomenon and assess whether similar mechanisms occur also in other grasshoppers. Understanding these interactions may provide insights into thermochromic biological systems and help determine whether the pigment–protein complex can be isolated and applied in bio-inspired sensing materials.

[1] Innes C. Cuthill et al., The biology of color. Science 357, eaan0221(2017). https://doi.org/10.1126/science.aan0221
[2] Bodo D. Wilts, Karolina Mothander, Almut Kelber; Humidity-dependent colour change in the green forester moth, Adscita statices. Biol Lett 1 September 2019; 15 (9): 20190516.
https://doi.org/10.1098/rsbl.2019.0516
[3] L.Wang, B. D.Wilts, Reversible Temperature Sensing using Blue-Winged Grasshopper Coloracris azureus Wings. Small 2024, 20, 2310193.
https://doi.org/10.1002/smll.202310193

371 **P040**	**Near-field to Far-field: Evolution of Optical Fields in Butterfly Distal Optics**	Mahdi Khodadadi Karahroudi	Poster

Mahdi Khodadadi Karahroudi (1) Primoz Pirih (1) Bodo Wilts (1)

(1) University of Salzburg

The compound eyes of butterflies consist of thousands of ommatidia, each functioning as a compact optical unit that precisely routes incident light through its distal optics. In each ommatidium, a corneal lens and a gradient-index crystalline cone guide light into the rhabdom, which acts as a photoreceptive waveguide. A fraction of the non-absorbed light is reflected by a basal reflector and relaunched toward free space as eyeshine. Here, we investigate how optical fields evolve as the light propagates through the distal optics. We examine how field transformations depend on wavelength, geometry, and refractive-index profiles, and assess potential directional symmetry of forward and backward propagation. The results clarify how the light entering the photoreceptors is shaped, and how the back-propagated fraction emerges as eyeshine, transitioning into free space from Fresnel to Fraunhofer diffraction regime.

NESY - Physics of Neutron and Synchrotron Radiation Sources

NESY – Session 1 (Thu 24, 10:30-12:45, Chair: Herwig Michor)			
ID	Title	Speaker	Type
184	**Peak Performance: What the Dancing Peaks in Operando Small-Angle X-ray Data Reveal About Charge Storage in MOF-Based Supercapacitors**	Malina Seyffertitz	Contributed talk (10:30-11:00)

Malina Seyffertitz (1,2) Chloe J. Balhatchet (1) Max V. Rauscher (2) Sebastian Stock (2) Gerhard Fritz-Popovski (2) Heinz Amenitsch (3) Alexander C. Forse (1) Oskar Paris (2)

(1) University of Cambridge
(2) Montanuniversität Leoben
(3) TU Graz

Understanding ion behaviour at electrified interfaces is central to improving electric double-layer capacitors (EDLCs), yet many molecular-scale charge storage mechanisms and specific electrode-electrolyte interactions remain incompletely resolved. Operando synchrotron techniques such as Small Angle X-Ray Scattering (SAXS) and X-Ray Diffraction (XRD) are powerful tools to probe ion behaviour in nanoporous electrodes under working conditions. However, in conventional activated carbon electrodes, the disordered pore structure gives rise to broad and complex scattering features, hindering a more direct interpretation and quantitative analysis. To enable more direct insight, we use an ordered metal-organic framework (MOF) as a model material, in which cylindrical nanopores arranged on a hexagonal lattice give rise to well-defined Bragg peaks, facilitating data interpretation.
Here, we investigate charge storage in the electrically conductive Ni3(HITP)2 MOF using a 1 M NaTFSI aqueous electrolyte. Operando SAXS measurements were performed at the Austrian SAXS beamline at Elettra, complemented by XRD measurements at the ID22 beamline at the European Synchrotron Radiation Facility (ESRF). Using this combined synchrotron approach, we show that TFSI- anions are immobilized near MOF pore walls via fluorine–hydrogen interactions with N-H functional groups at the electrode. We quantify the concentration of pinned anions and demonstrate that their immobilisation persists across applied cell voltages, resulting in a cation-dominated charge storage mechanism governed solely by Na+ adsorption and desorption.
These findings reveal how combining operando synchrotron techniques with a well-defined model system enables direct insight into interfacial ion behaviour, enabling a mechanistic explanation for the cation-dominated charge storage observed in many MOF-based systems. More broadly, this work establishes a framework for understanding ion electrosorption during electric double-layer formation in aqueous supercapacitors, enabling the targeted design of charge storage mechanisms through controlled interfacial interactions.

516	**Analysis of PERKEO III**	Alberto José Saavedra García	Contributed talk (11:00-11:15)

Alberto José Saavedra García (1)

(1) Technische Universität Wien - Atominstitut

Precision measurements of free neutron decay provide a powerful probe of the Standard Model and potential physics beyond it (BSM). Experiments such as PERKEO III and PERC are designed to study neutron beta decay with unprecedented accuracy by analyzing correlations among decay products.
PERKEO III has delivered the most precise measurement of the beta asymmetry parameter A, from which the most precise determination of λ is obtained. Being this ratio between the axial-vector and vector coupling constants (λ=g_A/g_V), λ plays a key role in determining the Cabbibo-Kobayashi-Maskawa (CKM) matrix element V_{ud} and thus in testing its unitarity.While PERC is designed to further improve this precision, it is still under construction. In the meantime, existing results can be further refined by reanalyzing the data with improved theoretical corrections and by achieving a better understanding of the dominant sources of systematic uncertainty.

748	**The HF-SAXS and HB-SAXS Beamlines at ELETTRA2.0**	Heinz Amenitsch	Contributed talk (11:15-11:30)

Heinz Amenitsch (1)

(1) Institute of Inorganic Chemistry, Graz University of Technology

Following the shutdown of ELETTRA, the former Austrian Small Angle X-ray Scattering (SAXS) beamline will be replaced by two new SAXS beamlines at the low-emittance storage ring ELETTRA 2.0, the upgrade program of Elettra Sincrotrone Trieste: the high-flux (HF) and high-brilliance (HB) SAXS beamlines.
This contribution presents the main design parameters and scientific case. The HF-SAXS beamline uses a 1.4 m long, 49-pole superconducting wiggler (3.5 T), accepting a radiation cone of 0.2 × 0.5 mrad at 0.75 mrad off-axis. It operates at a fixed energy of 10.4 keV, monochromatized with a cryo-cooled Si (111) crystal at 16.5 m. A fixed-focus, 850 mm long toroidal mirror focuses the beam to 36.5 m. With a maximum sample-to-detector distance of 4 m, a beam size of ~1.5 × 0.4 mm^2 and a flux of ~5×10^{12} ph/s are achieved, with a SAXS resolution of ~300 nm. Applications include high-throughput SAXS/GISAXS in structural biology, materials science, and slow dynamics. Commissioning is planned for early 2027.
The HB-SAXS beamline employs a 2 m in-vacuum undulator (109 poles, 5.2 mm gap), delivering 4.5–17 keV radiation within a 40 µrad × 40 µrad cone. A dual monochromator (Si (111) and multilayer) combined with Kirkpatrick–Baez mirror optics enables variable focusing between 32 and 38 m. The beam size is ~0.2 × 0.13 mm^2, with a flux of 10^{12}–10^{14} ph/s and SAXS resolution better than 500 nm. This branch targets fast structural transitions; reflectivity and simultaneous X-ray spectroscopy are under evaluation.The mirrors can be removed to provide highly coherent radiation for photon correlation spectroscopy. Future upgrades include secondary optics to achieve ~5 µm spot size for 3D tensor SAXS and scanning SWAXS. Commissioning of the first part is planned for late 2027.

453	**Synchrotron X-ray Scattering Studies following in-situ the Temperature Dependent Aggregation States of 1D fibrils**	Rainer T. Lechner	Contributed talk (11:30-11:45)

Rainer T. Lechner (1) Philipp Schwarz (1) Amelia Cedrowicz (2) Thai Hai Luong (2) Klaus Boldt (2)

(1) Montanuniversität Leoben, Austria
(2) Universität Rostock, Germany

In this work, we analyze a 1-dimensional, atomically defined, phosphonate-capped CdSe nanomaterial using in-situ SAXS/WAXS at the P62 beamline at DESY combined with anomalous SAXS and x-ray absorption (XAS) close to the Se edge. The structure is related to the class of magic-size clusters that form in the early stages of nanocrystal synthesis and play a pivotal role in anisotropic growth of colloidal nanorods [1, 2].
The material forms a colourless gel at room temperature and melts into individual fibrils that are stable up to 310 °C. The change in the aggregation state from aggregated bundles of fibrils at room temperature to individual fibrils was studied in real time by SAXS/WAXS measurements. With this we could reveal the separation of the bundles above 60 °C and could follow the transformation to separated 1D fibrils with a diameter of only ~2 nm and above 100 nm in length. This is achieved, e.g., by analysing the slope of the SAXS intensity at low q as a function of temperature.
The small diameter of the fibrils is related to the formation of magic size clusters [3] that merge along the rotational axis into a continuous, inorganic material with a helical structure. This rod formation is only initiated by the use of a phosphonate based ligand, whereby a pure oleic acid ligand does not lead to a homogenous rod formation.
From standard SAXS analysis we found, however, that the diameter determination of the CdSe fibrils is influenced by the phosphonate shell. Thus, anomalous SAXS (ASAXS) measurements are required for retrieving the pure CdSe dimensions that can be then compared to magic-sized CdSe clusters [4].

[1] D. Wurmbrand, at al., & K. Boldt, Chem. Commun. 2018, 54, 7358.
[2] D. Fischli, F. Enders, K. Boldt, J. Phys. Chem C 2020, 124, 12774.
[3] C. B. Williamson, at al., & R. D. Robinson, Science 2016, 363, 731.
[4] K. Boldt, et al., & P. Schwarz, R.T. Lechner, to be submitted 2026

454	**Small Angle X-ray Scattering and Visible Spectroscopy Studies of Photoactive Systems using a Tailored Microfluidic Device**	Benedetta Marmiroli	Contributed talk (11:45-12:00)

Benedetta Marmiroli (1) Sumea Klokic (1) Barbara Sartori (1) Alessio Turchet (2) Marie Reissenbuechel (1) Heinz Amenitsch (1)

(1) Institute of Inorganic Chemistry, Graz University of Technology
(2) Elettra-Sincrotrone Trieste

Microfluidic devices are increasingly employed in synchrotron experiments to enhance the study of liquid samples. However, few are designed for simultaneous photoexcitation and X-ray scattering, which is crucial for understanding rapid structural transitions of photoactive systems (molecules which undergo reversible structural changes among two or more isomeric forms, using light for at least one direction of switching [1]). This work presents a novel microfluidic device that is transparent to X-rays in a direction and to UV and visible light in the perpendicular one, enabling photo switching experiments where UV/visible laser light is the pump, and X-rays are the probe. The device is fabricated by a simple sequence of lamination and optical lithography steps on a dry film resist, and does not necessarily require a clean room facility. The effective study of photoactive systems and the device capability for time-resolved structural studies are demonstrated through successful experiments with hemoglobin and azobenzene derivatives [2]. These measurements further open the possibility for future investigations of laser induced T-jumps and pump probe experiments using synchrotron SAXS.

[1] A. W. A. Velema, J. P. Van Der Berg, M. J. Hansen, W. Szymanski, A. J. M. Driessen and B. L. Feringa, Nat Chem, 2013, 5, 924-928.
[2] B. Marmiroli, S. Klokic, B. Sartori, M. Reißenbüchel, A. Turchet, and H. Amenitsch, Lab on Chip (2026), DOI: 10.1039/D5LC01116G

141	**Characterization of Power and Spatial Beam Properties at the PTB DWL20 Synchrotron Beamline**	Hans Kirschner	Contributed talk (12:00-12:15)

Hans Kirschner (1) Michael Kolbe (1) Chistian Laubis (1) Jana Puls (1) Frank Scholze (1) Thomas Wiesner (1)

(1) Physikalisch-Technische Bundesanstalt

Controlled irradiation with synchrotron radiation requires precise knowledge of beam power and spatial intensity distribution. We present a comprehensive characterization of the PTB white light beamline DWL20 at BESSY II. The beamline utilizes direct radiation from a dipole bending magnet, focused by a Rh-coated ellipsoidal mirror and spectrally shaped using selectable filter configurations.
A calibrated CCD camera was employed to determine both the total beam power and the spatial beam profile at various distances from the focal point. The CCD was previously calibrated at the PTB EUV beamline, enabling a quantitative conversion of measured count rates into absolute power values. Measurements for different filter setups allow adjustment of the beam power.
The spatial analysis reveals a linear dependence of the beam width on the distance from the focus. Further, the beam structure shows a pronounced intensity peak and a broader homogeneous region. Based on this, the beam was systematically separated into a spot with high intensity and one with low intensity.
Combining total power measurements with spatial intensity distributions enables the determination of power densities for both regions as a function of focal position. The results provide a consistent and quantitative description of the DWL20 beam properties and form a reliable basis for reproducible irradiation experiments.

633	**Absolute Configuration Assignment from a Single Reflection using Resonant X-ray Diffraction**	Anmol Andotra	Contributed talk (12:15-12:30)

Anmol Andotra (1) Roland C. Fischer (1) Fabian Gasser (1) Yves Geerts (2,3) Ferdinando Malagreca (4) Roland Resel (1)

(1) Institute of Solid State Physics, Technical University of Graz
(2) Free University of Brussels (ULB)
(3) International Solvay Institutes
(4) Université Libre de Bruxelles

Chirality has become increasingly significant across a range of disciplines, including chemistry, materials science, biology, and the pharmaceutical industry. Resonant (anomalous) X-ray scattering provides a direct method for probing chirality in crystals. By tuning the incident energy near atomic absorption edges, resonant scattering breaks the symmetry between lattice planes (−h −k −l) and (h k l), known as Friedel's law, by introducing a measurable intensity difference between Friedel pairs. This principle has been well established in single crystal X-ray diffraction (SCXRD) for assigning absolute configuration using the Flack parameter. However, in many experimental geometries, such as grazing incidence X-ray diffraction (GIXD), access to complete Friedel pairs is restricted. This talk presents a new approach for assigning the absolute configuration of enantiomorphic chiral crystals of the Br-oxo molecule. Simulations of the energy-dependent structure factors for different reflections show distinct energy dependences for the two absolute configurations, whereas others remain identical. By comparing the measured and simulated energy dependent intensities, the absolute configuration can be assigned using the intensity of a single reflection, even in cases where conventional approaches rely on multiple Friedel pairs. This approach opens new opportunities for studying chiral crystals and offers potential extensions to thin-film systems.

404	**Spin-Pumping and Induced Magnetic Polarization in Permalloy/ Platinum Heterostructures**	Verena Ney	Contributed talk (12:30-12:45)

Fabian Ganss (1) Réne Hübner (1) Kilian Lenz (1) Jürgen Lindner (1) Andreas Ney Verena Ney (2) Andrei Rogalev (3) Fabrice Wilhelm (3)

(1) Helmholtz-Center Dresden-Rossendorf
(2) Johannes Kepler University Linz
(3) ESRF Grenoble

Spin pumping is the transfer of angular momentum across interfaces into a non-ferromagnetic material driven by the precessing magnetization of an adjacent ferromagnet. Using ferromagnetic resonance (FMR) the presence of spin pumping can be evidenced by an increase of the Gilbert damping parameter α [1]. Here we study Platinum-Permalloy (Pt/Py) heterostructures using temperature-dependent broadband FMR. A clear increase of α is seen in a temperature range from 10-300 K when Pt and Py are in direct contact. The temperature dependence of the spin-pumping contribution can be derived by comparing with an Al-sandwiched Py reference film from [2]. Surprisingly, upon insertion of a thin Al spacer layer between Pt and Py the increase in α is suppressed. X-ray magnetic circular dichroism at the Pt L-edge reveals a clear magnetic polarization in Pt/Py whereas it is absent when a spacer layer of only 2 nm of Al is inserted. The induced polarization of Pt can thus be associated with spin pumping, while non-polarized Pt in proximity to Py shows an almost identical $\alpha(T)$ behavior as the Py reference sample in [2].

[1] Y. Tserkovnyak Phys. Rev. Lett. 88, 117601 (2002)
[2] V. Ney et al. Phys. Rev. Materials 7, 124403 (2023)

NESY – Session 2 (Thu 24, 16:00-18:15, Chair: Andreas Ney)			
ID	Title	Speaker	Type
	Introduction		(16:00-16:15)
789	**Fourth Generation Synchrotron Sources: A Quantum Leap for Matter Exploration. The Example of the ESRF Extremely Brilliant Source**	Jean Daillant	Invited talk (16:15-16:45)

Jean Daillant (1)

(1) European Synchrotron Research Facility, Grenoble

The ESRF-EBS exemplifies how next-generation synchrotron sources open unprecedented avenues for probing the structure and dynamics of matter, driving breakthroughs across physics, chemistry, biology, and materials science. In 2020, the ESRF, where 19 partner countries join forces to exploit 46 cutting edge beamlines at the forefront of synchrotron technology completed the upgrade of its storage ring. The upgrade boosted the source's brilliance and coherence by two orders of magnitude, enabling experiments that were previously impossible to perform. New capabilities include: i) hierarchical imaging spanning from 10 nm up to the meter scale, ii) Dynamic-process studies ranging from 100 ps to months, capturing ultrafast phenomena and long-term evolution, iii) elemental - composition sensitivity at the ppb level, iv) high-throughput characterization, allowing hundreds of samples to be analysed in minutes. I will present recent ESRF studies that highlight the transformative impact of fourth-generation synchrotrons. I will also briefly discuss short and long term plans for the further development of the facility.

680	**Spatiotemporal Nanoscale Strain Analysis of Functional Materials at ESRF and PETRA III**	Jozef Keckes	Invited talk (16:45-17:15)

Jozef Keckes (1)

(1) Montanuniversität Leoben

Functional materials possess complex strain gradients that critically influence the performance characteristics of the technological components they constitute. These gradients may originate (i) from intentionally applied processing conditions, (ii) from self-organized phenomena, and/or (iii) from inhomogeneous thermal or mechanical loads experienced during service. To optimize component performance, it is essential to quantitatively assess strain gradients at the nanoscale and their evolution during operation. In this contribution, I will present experimental findings obtained by my group at the ID13 and ID03 beamlines of ESRF and the P07B beamline at PETRA III.
Cross-sectional synchrotron X-ray nanodiffraction (CSnanoXRD) [1], utilizing monochromatic X-ray beams with diameters down to ~25 nm, provides spatially resolved insights into the evolution of phases, crystallographic texture, grain morphology, and strain/stress distributions in nanocrystalline materials. I will discuss the methodological and instrumental aspects of the approach and highlight recent studies performed at the ID13 beamline. Examples will include thin films, nanomaterials and battery systems, with particular emphasis on in situ experiments and the analysis of complex depth gradients in microstructure–strain–property relationships [2,3].
Subsequently, strain characterization by dark-field X-ray microscopy (DFXM) at the ID03 beamline will be addressed. DFXM was employed to study Cu metallizations, revealing the origins of microscopic void and crack formation at high-angle grain boundaries (HAGBs). This behaviour is attributed to vacancy condensation in front of HAGBs, following dislocation motion across cyclically deformed grains. The observed HAGB decohesion correlates with local hardening near grain boundaries, as evidenced by X-ray diffraction peak broadening and elastic strain accumulation [4,5]. In addition, DFXM investigations of solid-state batteries—specifically dendrite growth in LLZO crystals—will be discussed [6].
Finally, recent high-energy X-ray diffraction studies of hydrogen–metal interactions, performed at the P07B beamline, will be presented. In situ experiments using custom electrochemical cells enabled us to elucidate the role of lattice swelling in the evolution of elastic strains, plastic deformation and hydride formation [7,8].

[1] Keckes et al., Acta Mat. 144 (2018) 862, https://doi.org/10.1016/j.actamat.2017.11.049
[2] Meindlhumer et al., Communications Materials 6 (2025) 35, https://doi.org/10.1038/s43246-025-00752-z
[3] Flatcher et al., Small 20 (2024) 2307515, https://doi.org/10.1002/smll.202307515
[4] Hlushko et al., Acta Mat. 253 (2023) 118961, https://doi.org/10.1016/j.actamat.2023.118961
[5] Ziegelwanger et al., npj Materials Degradation 9 (2025) 79, https://doi.org/10.1038/s41529-025-00629-z
[6] Yildirim et al., Nature Communications 15 (2024) 8207, https://doi.org/10.1038/s41467-024-52412-4
[7] Weiser et al., Acta Mat. 277 (2024) 120217, https://doi.org/10.1016/j.actamat.2024.120217

[8] Pogrielz et al., Corrosion Science 257 (2025) 113282, https://doi.org/10.1016/j.corsci.2025.113282

786	**A Hybrid Machine Learning and Atomistic Modeling Approach for the Design of de novo Enzymes**	Gustav Oberdorfer	Invited talk (17:15-17:45)

Gustav Oberdorfer (1)

(1) Institute of Biochemistry, Graz University of Technology, Petersgasse 12/2, A-8010 Graz, Austria

Reliably introducing function into genetically encodable de novo proteins is still a challenging task. Current design methods mostly produce de novo enzymes with low activities. As a result, they require costly experimental optimization and high-throughput screening to be industrially viable. We developed rotamer inverted fragment finder–diffusion (Riff-Diff), a hybrid machine learning and atomistic modelling strategy for scaffolding catalytic arrays in de novo protein backbones. We show that proficient enzymes can be generated with Riff-Diff while screening as little as 35 designs. Easy access to synchrotron beamlines at the ESRF enabled us to screen several hundred protein crystals and led to the determination of six protein structures of our de novo enzymes. These experimental structures revealed a counterintuitive correlation between design accuracy and catalytic activity, which I will highlight during the talk.

513	**Structure and Relaxation Dynamics of Ionic Liquid at Interfaces and in Confinement**	Markus Mezger	Contributed talk (17:45-18:00)

Markus Mezger (1)

(1) University of Vienna

Ionic liquids (ILs) composed of cations with long aliphatic side chains can exhibit mesoscopic order and liquid crystalline mesophases. The solvate affinity to the ionic- and aliphatic domains of such ILs can strongly affect their interfacial structures. We employ X-ray scattering techniques to investigate these structures on the molecular length scale in bulk, near surface and in nm-confinement. Synchrotron experiments were performed at ESRF and PETRAIII. Here, we present results from neat ILs and IL/solvent mixtures. At the surface, we observe the formation of adsorbate layers and surface induced smectic order. In confinement we follow the adsorption/desorption dynamics and structural relaxation processes.

538	**Quantifying Nanoscale Electrochemical Conversion Through Machine Learning-Assisted Operando Small-Angle Scattering**	Christian Prehal	Contributed talk (18:00-18:15)

Christian Prehal (1)

(1) Department of Chemistry and Physics of Materials, University of Salzburg, Jakob-Haringer-Straße 2a, 5020 Salzburg, Austria

Operando synchrotron and neutron techniques have become indispensable tools for resolving the structural and chemical complexity of electrochemical phase transformation in battery materials. In this talk, I present how operando SAXS/WAXS and SANS, combined with machine learning-assisted stochastic modelling, can quantify conversion mechanisms in post lithium-ion batteries at length scales difficult to access with other techniques.
The central focus is lithium-sulfur (Li-S) batteries, where the transformation between solid sulfur and solid lithium sulfide largely defines battery performance and can proceed through solid-liquid-solid, quasi-solid-state, or solid-state pathways depending on electrolyte and cathode composition. I present results tracking the growth and dissolution of solid deposits at nanometer scales across these different regimes [1-3]. Combined with cryo-transmission electron microscopy, the data show that the deposit consists of nanocrystalline Li_2S alongside smaller solid short-chain polysulfide particles. These findings inform strategies for controlling the reaction pathway in next-generation Li-S cells.
As a second example, I will discuss how related approaches apply to sodium-ion batteries, where hard carbon anode sodiation and desodiation mechanisms are resolved at the nanoscale. I will present preliminary work on active Bayesian learning for scattering-based quality control of hard carbon synthesis, with relevance to process optimisation in practical materials manufacturing.

[1] C. Prehal, V. Wood et al., Nature Communications 2022, 6326
[2] J.-M. von Mentlen, C. Prehal et al., ACS Nano 2025 19, 16626
[3] P. Dutta, C. Prehal et al., ACS Energy Letters 2025, 10, 5722

NESY – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
60 **P095**	**Finding Crystal Orientation in Uniplanar Textures**	Josef Simbrunner	Poster

Josef Simbrunner (1) Fabian Gasser (2) Sanjay John (2) Roland Resel (2)

(1) Medical University Graz
(2) Institute of Solid State Physics, TU Graz

The crystallization of molecular materials on isotropic substrates typically results in a so-called fiber or uniplanar texture which comprises crystallites that share a common fiber axis perpendicular to the substrate surface, but which are azimuthally randomly oriented. The crystallographic characterization of such films is performed by grazing-incidence X-ray diffraction (GIXD). Two-dimensional reciprocal space maps are obtained, which incorporate the in-plane component qxy and the out-of-plane component qz for each diffraction peak. The exact position of each diffraction peak depends on the crystallographic lattice and on the orientation of the unit cell relative to the substrate surface. The unit cell orientation can be characterized either by two rotation angles or by the Miller indices of the crystallographic plane parallel to the substrate surface. Equations are derived that allow the calculation of the orientation parameters and describe the relations between them. Dependent on the underlying unit cell, a manifoldness of possible orientations exists. Examples based on molecular crystals of pentacenequinone, diindenoperylene and binaphthalene are given which are illustrative examples comprising triclinic, monoclinic and tetragonal unit cells which have two, four and 16 possible crystal orientations, respectively.

301 **P096**	**Crystalline Electric Field Studies of $RNiC_2$**	Danny Milosavljevic; Herwig Michor	Poster

Danny Milosavljevic (1) Marta Roman (1) Devashibhai T. Adroja (2) Herwig Michor (1)

(1) Institute of Solid State Physics, TU Wien
(2) ISIS Neutron Facility

Ternary carbides $RNiC_2$ (R = rare earths and Y) crystallize in the non-centrosymmetric orthorhombic $CeNiC_2$-type structure, space group Amm2. This family of compounds attracted attention, because of interesting properties such as superconductivity, magnetism, multiple charge density wave (CDW) transitions related to quasi-one-dimensional electronic features, and finally, a complex interplay of CDW order and rare earth magnetism (see Ref. [1] for a review). Here, we report on studies of the crystalline electric field effects in $RNiC_2$. Single crystal data of thermodynamic bulk properties such as heat capacity and magnetic susceptibility of heavy rare earth $RNiC_2$ with R = Tb-Tm are complemented with powder inelastic neutron scattering studies of $DyNiC_2$ and $TmNiC_2$ conducted at the MAPS instrument at the ISIS neutron spallation source to analyse the crystalline electric field (CEF) splitting in these compounds in terms of a systematic evolution of corresponding universal CEF parameters. The latter are essential to further explore the formation of magnetic ground states of these compounds.

[1] V. Babizhetskyy, B. Kotur, V. Levytskyy, H. Michor, Chapter 298: Alloy systems and compounds containing rare earth metals and carbon, in: J.-C.G. Bünzli, V.K. Pecharsky (Eds.), Handbook on the Physics and Chemistry of Rare Earths, Vol. 52, North-Holland, Amsterdam, pp. 1-263. (2017).

729 **P097**	**Nanoscale Investigation of Heavy Metal Uptake in Two Bryophytes by Simultaneous nano-SRXRF and SAXS**	Matthias Weinberger	Poster

Matthias Weinberger (1) Sebastian Kalbfleisch (2) Ingeborg Lang (3) Helga Lichtenegger (1) Luigi Schillaci (3)

(1) Institute of Physics and Materials Science, BOKU
(2) NanoMax, MAX IV Laboratory
(3) Department of Functional and Evolutionary Ecology, University of Vienna

Bryophytes are highly efficient sorbents of nutrients and metals, making them powerful biomonitors and model systems for studying plant metal uptake. We investigate metal distribution and ultrastructural responses in two mosses, Physcomitrium patens and Pohlia drummondii. The latter is known for its heavy metal tolerance, potentially attributable to its thick cell walls. Specimens were grown under controlled metal exposures in the laboratory.
Using nano-Synchrotron X-ray Fluorescence (nano-SRXRF) combined with simultaneous Small-Angle X-ray Scattering (SAXS) at the NanoMAX beamline at MAX IV, we mapped subcellular distributions of “housekeeping” elements (Cl, Ca, K) and contaminant metals (Fe and Cu) to assess their effects on cellular ultrastructure. We employ the Compton signal for normalization and quantification, enabling conversion from areal to volume concentrations. This allows direct comparison with the metal exposure from the agar and across scans.
At NanoMAX, the nano-focused beam and high brilliance reveal nanoscale elemental heterogeneity, which was not seen with lower resolution. We resolve previously unreported iron nanoclusters within bryophyte tissues. SAXS probes potential metal induced modifications of the cell wall, allowing us to test whether exposure produces detectable changes in scattering signatures associated with wall alterations

496 **P098**	**In situ Phase-Contrast Microtomography Experiments at the BEATS Beamline of the SESAME Synchrotron**	Fareeha Hameed	Poster

Fareeha Hameed (1) Ahmed Wagih Abdelhady (2) Mehmet Nurullah Ates (3) Ali Karatutlu (4) Petra Julia Koch (5) Hassan Mahmoud (2) Andreas Staude (5)

(1) SESAME Synchrotron, Jordan
(2) KAUST (King Abdullah University of Science and Technology), Saudi Arabia
(3) Bogazici University, Turkey
(4) National Nanotechnology Research Center (UNAM) and Institute of Materials Science Nanotechnology, Bilkent University, Ankara 06800, Turkey
(5) Charite Universitatsmedizin Berlin, Germany

3D X-ray imaging is a powerful technique. Over time, great progress has been made in terms of the spatial and temporal resolution. Synchrotron radiation has properties of high flux, brightness, and stability required for fast imaging. The ID10 - BEATS beamline at the SESAME synchrotron is a microtomography beamline. Advanced imaging techniques include phase-contrast microtromography and edge-sensitive imaging. This beamline is relatively new, starting its operation in 2024. Successful in situ experiments have been performed. These include mechanical testing, tensile and compression tests, battery charging and discharging, and fluid flow experiments. Further experiments are being designed for in situ induction heating. A new sample stage is being installed and commissioned. These developments and initial user experiments illustrate the capabilities of the BEATS beamline regarding time-resolved measurements, which is a state-of-the-art method.

[1] www.sesame.org.jo/beamlines/beats
[2] Fedele R, et al. J Imaging 7(11):240, 2021.
[3] Karatutlu A, et al. Conf Lasers Electro-Optics/Europe (CLEO/Europe 2025)
[4] Virazels T, et al. SSRN, 5668575.
[5] Bidola P, et al. J Synchrotron Radiat. 33(1), 2026.
[6] Rogalinski JK, et al. J Synchrotron Radiat. 33(2), 2026.
[7] Prajapati A, et al. Nat Commun. 16(1):2593, 2025.

OeAW – Young Academy of the Austrian Academy of Sciences

OeAW – Session 1 (Thu 24, 10:30-12:30)			
ID	Title	Speaker	Type
81	**Molecular Assembly and Coupling on Surfaces: From Electrostatics to Heterocyclic Systems**	Laerte Patera	Invited talk (10:30-11:00)

Laerte Patera (1)

(1) Universität Innsbruck

Understanding the intricate mechanisms governing molecular assembly and coupling on surfaces is essential for advancing surface chemistry and nanotechnology. Here, I will present an exploration of phenomena ranging from electrostatic interactions to the formation of heterocyclic systems, exploiting high-resolution scanning probe microscopy.
The first part will focus on dihydrogen bonding (DHB), a distinctive intermolecular interaction where hydrogen atoms simultaneously act as proton donors and acceptors. Low-temperature scanning tunneling microscopy (LT-STM) reveals single and double DHB motifs within borazine assemblies on Au(111) surfaces. Complementary density functional theory (DFT) calculations provide critical insights into the interplay between substrate adsorption and intermolecular forces, elucidating the stabilization mechanisms driving the formation of borazine clusters.
The second part will examine the self-assembly of fullerene C60 and Zn(II)-5,10,15,20-tetrakis(4-aminophenyl)porphyrin (ZnTAPP) on a Ag(111) surface. Kelvin Probe Force Microscopy (KPFM) and Scanning Tunneling Spectroscopy (STS) unveil the intricate role of charge transfer and Coulomb interactions in shaping intermixed molecular phases. Notably, the alleviation of repulsive inter-fullerene Coulomb forces promotes the formation of row-like structures, which, in turn, enhance charge transfer to C60 molecules. These findings highlight the delicate balance between substrate-mediated electron transfer and intermolecular forces in directing molecular self-assembly.
The final part will demonstrate the on-surface synthesis of nitrogen-containing heterocycles, which are fundamental building blocks in biomolecules and pharmaceuticals. Thermal activation of a tailored precursor leads to the formation of an N-heterocyclic compound, as visualized by high-resolution non-contact atomic force microscopy (nc-AFM). DFT calculations reveal the reaction mechanism, emphasizing the critical role of hydrogen release as the driving force behind the transformation.

105	**Adventitious Carbon Breaks Symmetry in Oxide Contact Electrification**	Scott Waitukaitis	Invited talk (11:00-11:30)

Scott Waitukaitis (1) Galien Grosjean (2) Markus Ostermann (3) Markus Sauer (4) Michael Hahn (5) Christian M. Pichler (5) Florian Fahrnberger (5) Felix Pertl (1) Daniel M. Balazs (1) Mason M. Link (6) Seong H. Kim (6) Devin L. Schrader (7) Adriana Blanco (8) Francisco Garcia (8) Nicolas Mujica (9)

(1) Institute of Science and Technology Austria
(2) Autonomous University of Barcelona
(3) Institute for Applied Physics, TU Wien
(4) Analytical Instrumentation Center, TU Wien
(5) Institute for Chemical Technology and Analytics, TU Wien
(6) Department of Chemical Engineering and Materials Research Institute, Pennsylvania State University
(7) Astromaterials Research and Exploration Science (ARES) Division, XI3 Research Office, NASA Johnson Space Center, Houston, TX
(8) Departamento de Ingeniería Química, Biotecnología y Materiales, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago
(9) Departamento de Física, Facultad de Ciencias Físicas y Matemáticas, Universidad de Chile, Santiago

Insulating oxides are among the most abundant solid materials in the universe. Of the many ways in which they influence natural phenomena, perhaps the most consequential is their capacity to transfer electrical charge during contact—which occurs even between samples of the same oxide—yet the symmetry-breaking parameter that causes this remains unidentified. Here we show that adventitious carbonaceous molecules adsorbed from the environment are the symmetry-breaking factor in same-material oxide contact electrification (CE). We use acoustic levitation to measure charge exchange between a sphere and a plate composed of identical amorphous silicon dioxide (SiO2). Although charging polarity is random for co-prepared samples, we control it with baking or plasma treatment. Observing the charge-exchange relaxation afterwards, we see dynamics over a timescale of hours and connect this directly to the presence of adventitious carbon with time-of-flight mass spectrometry, low-energy ion scattering and infrared spectroscopy. Going further, we confirm that adventitious carbon can even determine charge exchange among different oxides. Our results identify the symmetry-breaking parameter that causes insulating oxides to exchange charge in settings ranging from desert sands to volcanic plumes, while simultaneously highlighting an overlooked factor in CE more broadly.

241	**Molecules in Fields and Solids: Topology, Control, and Many-Body Physics**	Mikhail Lemeshko	Invited talk (11:30-12:00)

Mikhail Lemeshko (1)

(1) Institute of Science and Technology Austria

I am going to tell you about new physical phenomena emerging in molecules interacting with fields, with one another, and with a solid-state environment.
First, I will show how topological physics can emerge even in a single diatomic molecule periodically driven by a laser pulse [1]. This paves the way to studying controllable topological physics in gas-phase experiments with small molecules as well as to classifying dynamical molecular states by their topological invariants.
Second, I will present our recent progress on interaction of molecules and clusters with light carrying orbital angular momentum [2], with applications to precision spectroscopy, rotational control and chiral discrimination of molecules.
Finally, I will present our recent attempts develop simple models to describe soft semiconductors containing rotating molecules, such as lead-halide perovskites known for their outstanding photovoltaic properties [3]. Turns out, a lot of physics observed in such complex materials can already be captured by very simple lattice models.

[1] V. Karle, A. Ghazaryan, M. Lemeshko, Phys. Rev. Lett. 130, 103202 (2023)
[2] M. Maslov, G. M. Koutentakis, M. Hrast, O. H. Heckl, M. Lemeshko, Phys. Rev. Research 6, 033277 (2024)
[3] F. Kluibenschedl, G. M. Koutentakis, R. Alhyder, M. Lemeshko Phys. Rev. Lett. 134, 096302 (2025)

603	**Tuning Magnetism in Graphene Moiré Heterostructures by Proximity-Induced Spin-Orbit Coupling**	Hryhoriy Polshyn	Invited talk (12:00-12:30)

Hryhoriy Polshyn (1)

(1) Institute of Science and Technology Austria

Narrow bands in graphene moiré heterostructures can host magnetic electronic states in which electrons become spontaneously valley-polarized due to strong electronic interactions. These magnetic states include both gapped states at integer superlattice fillings that manifest the quantized anomalous Hall effect (QAHE), and metallic states that exhibit the anomalous Hall effect (AHE) at intermediate fillings. A ubiquitous feature of such magnetic states is the presence of magnetization reversal points, where the magnetization changes sign as a function of chemical potential, displacement field, or other control parameters. Such reversal points enable non-volatile electrical manipulation of the magnetic states, providing a useful control knob for potential devices based on AHE or QAHE phases.
Proximity-induced spin–orbit coupling provides a promising route to engineer the magnetic properties of graphene moiré systems, as it controls the interplay between the orbital and spin contributions to the magnetization. I will present a systematic study of gapped and metallic ferromagnetic states in twisted monolayer–bilayer graphene (tMBG) devices proximitized with WSe_2. I will discuss the details of the onset of the quantized anomalous Hall plateau in these devices. Finally, I will examine how proximity-induced spin–orbit coupling affects non-volatile electrical switching in this system.

OGD - Surfaces, Interfaces and Thin Films

OGD – Session 1 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
644	**Atomically Defined On-Surface Synthesis of Multilayer Metal-Organic Frameworks**	Zdenek Jakub	Contributed talk (16:00-16:15)

Zdenek Jakub (1) Jakub Planer (1) Dominik Hrůza (1) Zdeněk Endstrasser (1) Pavel Procházka (1) Jan Čechal (1)

(1) CEITEC - Central European Institute of Technology, Brno University of Technology

Solvent-free on-surface synthesis approach allows to design and study new materials with unrivaled resolution, but it is traditionally limited to materials of monolayer thickness. Here, we demonstrate that multilayer metal-organic frameworks (MOFs) can be grown on surfaces in ultrahigh vacuum, and these materials can be characterized at the atomic-scale using the established surface science methodology. By Scanning Tunneling Microscopy, Low Energy Electron Diffraction and X-Ray Photoemission Spectroscopy combined with Density Functional Theory computations, we show that an on-surface prepared multilayer Fe-TCNQ MOF structure is well-defined at the atomic scale, and features both in-plane and out-of-plane chemical bonding. The interlayer chemical interaction affects the structural and electronic properties of the material, making this system distinct from the monolayer case, and comparable to the materials studied in applied materials chemistry.
The multilayer growth is partially independent of the support, as we demonstrate its feasibility on two substrates: Au(111) and graphene/Ir(111). However, the support defines the growth mode of the MOF, which is Volmer-Weber (island) on graphene/Ir(111) and Stranski-Krastanov (layer-plus-island) on Au(111). We rationalize these observations by the different interaction strengths between the MOF components and the supports. Despite these differences, MOF thicknesses up to 3-4 monolayers were achieved on both supports, with no hints of any issues that would prevent growth of thicker structures. Overall, our results bridge the gap between fundamental atomically-resolved models and application-relevant materials.

738	**Computational Insight into CO Binding at On-Surface 2D MOFs: Fe–N_3 versus Fe–N_4 Single-Atom Sites**	Jakub Planer	Contributed talk (16:15-16:30)

Jakub Planer (1) Dominik Hruza (1) Ayesha Jabeen (1) Zdenek Jakub (1) Tadeáš Lesovský (1) Jan Čechal (1)

(1) CEITEC - Central European Institute of Technology, Brno University of Technology

Understanding what controls the reactivity of single-atom catalyst sites remains a central challenge in heterogeneous catalysis. In this contribution, I will address this question from the computational perspective using atomically defined Fe–N_3 and Fe–N_4 model sites embedded in on-surface prepared two-dimensional Fe-DCA and Fe-TCNQ metal–organic frameworks on graphene.
The Fe–N_3 and Fe–N_4 sites in Fe-DCA and in Fe-TCNQ are electronically very similar prior to adsorption: both exhibit a high-spin Fe^{2+} configuration with S = 2, and their d-orbital occupancies and energetic positions relative to the Fermi level are nearly identical. Nevertheless, density functional theory predicts a difference in CO adsorption energy of more than 0.6 eV, in agreement with atomically resolved scanning tunneling microscopy experiments.
I will show that this reactivity difference originates from the different structural response of the two coordination environments upon adsorption. The more flexible Fe–N_3 site can relax out of the N plane, enhancing Fe $3d_{xz/yz}$–CO $2\pi^*$ back-donation and stabilizing CO binding. These results demonstrate that coordination geometry controls reactivity not only through electronic structure, but also through structural adaptability, highlighting a limitation of purely electronic descriptors.

215	**Dynamic Behavior and Functional Responses in Stimuli-Responsive Metal-Organic Frameworks**	Sumea Klokic	Contributed talk (16:30-16:45)

Sumea Klokic (1)

(1) Technische Universität Graz

Designing switchable metal-organic frameworks (MOFs) that respond to external stimuli (e.g., light, temperature, or guest molecules) offers significant opportunities to control their properties in advanced applications such as energy storage and conversion, gas capture and release, or regulated molecular transport. External triggers can induce a wide spectrum of responses, ranging from reversible structural transformations and adsorption-desorption cycles to photo-induced changes enabled by targeted chemical design. [1,2] Despite this potential, achieving finely tuneable and predictable responsive behaviour in MOFs,particularly in the solid state, remains a central challenge. Addressing this requires a comprehensive understanding of how these materials respond under stimulation, including not only the nature and magnitude of structural changes, but also their reversibility, kinetics, and characteristic timescales.
In this context, the dynamic behaviour of stimuli-responsive MOFs across different forms and environments is investigated using a model system. The presented results illustrate how structural evolution under external stimuli is closely linked to framework geometry, flexibility, and chemical composition, which together govern the type, extent, and dynamics of the response.[1-5] These insights provide a basis for identifying general design principles for MOFs with controllable and adaptable switching behaviour, supporting the rational development of responsive framework materials.

[1] Klokic, S.; Marmiroli, B.; Birarda, G.; Lackner, F.; Holzer, P.; Sartori, B.; Abbasgholi-NA, B.; Dal Zilio, S.; Kargl, R.; Stana Kleinschek, K.; Stani, C.; Vaccari, L.; Amenitsch, H. Nat Commun 2025, 16 (1), 7135.
[2] Marmiroli, B., Klokic, S., Sartori, B., Reissenbuechel, M., Turchet, A., Amenitsch, H.; Lab on a Chip, 2026, Advance Article.
[3] Klokic, S., Naumenko, D., Marmiroli B., Carraro, F., Linares Moreau, M., Dal Zilio, S., Birarda, G., Kargl, R., Falcaro, P., Amenitsch, H., Chem. Sci., 2022, 13, 11869-11877.
[4] Klokic, S.; Marmiroli, B.; Naumenko, D.; Birarda, G.; Dal Zilio, S.; Velásquez-Hernández, M. D. J.; Falcaro, P.; Vaccari, L.; Amenitsch, H. CrystEngComm 2024, 26 (17), 2228.
[5] Afanasenko, E., Marmiroli, B., Abbasgholi-NA, B.; Birarda, G., Stani, C., Finšgar, M., Hartmann, P. E., Bieber, M., Walitsch, E., Breinbauer, R., Dal Zilio, S., Klokic S. and Amenitsch, H., arXiv, DOI: 10.48550/arXiv.2603.24320.

688	**Influence of the Metal Ion on the Metal-Phthalocyanine Adsorption on Indium Oxide**	Viktoria Waidbacher	Contributed talk (16:45-17:00)

Viktoria Waidbacher (1) Matthias Blatnik (1) Ulrike Diebold (1) Michael Schmid (1) Margareta Wagner (1)

(1) Institute of Applied Physics, TU Wien, Austria

The interaction of conjugated organic molecules with oxide surfaces is of fundamental interest and relevant for applications ranging from optoelectronics to model catalysis. While organic/metal interfaces are well studied, the behavior on the transparent conductive oxide In_2O_3 remains comparatively unexplored. We investigate the adsorption of metal phthalocyanines (MPc) and metal free phthalocyanine (H_2Pc) on In_2O_3(111) using low temperature scanning

tunneling microscopy (STM), non contact atomic force microscopy (nc AFM), and density functional theory (DFT). The comparable size of the molecules and the surface unit cell enables a (1×1) arrangement despite symmetry mismatch (4 fold rotational symmetry of the molecule vs. 3 fold surface symmetry). Across different MPc species (CuPc, CoPc, etc.), we identify a common, robust adsorption site that enforces molecular overlap in the first layer, and a less frequent site that allows non overlapping (1×1) packing. Including H_2Pc reveals how the macrocycle interacts with the oxide in the absence of a metal center, providing a reference for understanding metal dependent adsorption. These insights link phthalocyanines to concepts in single atom catalysis: the Pc macrocycle stabilizes isolated metal atoms in a well defined N_4 pocket. Our results highlight how oxide surfaces—and by extension carbon–nitride like motifs—may offer more robust platforms for stabilizing single metal atoms, bridging molecular model systems and extended SAC materials.

617	**Infrared and Photoemission Spectroscopic Investigation of Small Copper Clusters and Their Oxidation States on Ag(100) and MgO/Ag(100) Surfaces**	Jacob Harrich	Contributed talk (17:00-17:15)

Jacob Harrich (1) Maximilian Laßhofer (1) Martin Sterrer (1)

(1) University of Graz, Institute of Physics

Transition metals such as copper (Cu) play a central role in heterogeneous catalysis and are widely used in industrial processes such as methanol synthesis. Stabilizing small Cu clusters or even isolated atoms on oxide supports is a common strategy to enhance catalytic performance. While magnesium oxide (MgO) is one of the best-characterized oxide materials, featuring well-defined, nonpolar surfaces and high stability, it is generally considered catalytically inert. Nevertheless, metal–support interactions can significantly alter the structural and electronic properties of supported metals, making MgO a suitable model system for fundamental studies.
This presentation covers thin-film and oxidation effects on Cu atoms and small clusters supported on MgO films grown on a silver single crystal Ag(100) under ultra-high vacuum conditions. MgO and Cu were deposited by e-beam evaporation. The system was characterized using Reflection-Absorption Infrared Spectroscopy (RAIRS), X-ray Photoelectron Spectroscopy (XPS) and complementary Scanning Tunneling Microscopy (STM). RAIRS provides insight into clustering behavior and charge state, while XPS was used to determine the oxidation state of Cu. STM measurements offer additional structural information on cluster morphology. The experiments with different Cu coverage and MgO films of various thicknesses demonstrate a complex nucleation behavior of Cu, ranging from single atoms and small clusters to three-dimensional particles. Additionally, differences in the oxidation and reduction behavior have been observed for small and large Cu particles. Interestingly, the oxidation of Cu on the surface of an ultrathin MgO film can also be achieved by the thermally induced diffusion of interfacial oxygen atoms, which form during the preparation of high workfunction MgO at the Ag/MgO interface. These results provide a comprehensive understanding of the metal-support interactions for Cu/MgO model catalysts.

613	**Seeding the Vertical Growth of Laterally Coherent Coordination Polymers on the Rutile-TiO_2(110) Surface**	Claudia Obersnu	Contributed talk (17:15-17:30)

Luca Schio (1) Gregor Bavdek (2) Cesare Grazioli (1) Claudia Obersnù (3) Albano Cossaro (4) Alberto Calloni (5) Alberto Bossi (6) Gianlorenzo Bussetti (5) Alessio Orbelli Biroli (7) Andrea Vittadini (8) Luca Floreano (1)

(1) CNR-IOM
(2) University of Ljubljana
(3) University of Graz
(4) University of Trieste
(5) Politecnico di Milano
(6) CNR-SCITEC
(7) University of Pavia
(8) CNR-ICMATE

The controlled fabrication of ordered molecular architectures with tailored functional properties at solid surfaces represents a key challenge for nanotechnology and device miniaturization. Although coordination polymers are efficiently obtained via conventional solution-based chemistry, their transfer onto substrates with the chemical, spatial, and geometrical homogeneity required for device integration remains challenging. Here, we adopt an in situ, vacuum-based, layer-by-layer self-assembly approach in which the anchoring sites are provided by ordered monolayers of metal(II)-tetraphenylporphyrins (M-TPP, M = Cu, Zn, Co) grown on the rutile TiO_2(110) surface. The metal center embedded in the porphyrinic macrocycle offers a well-defined coordination environment, enabling selective axial binding of a second-layer ligand. The affinity of the different metal ions toward axial coordination is investigated by subsequent deposition of symmetric dipyridyl-naphthalenediimide (DPNDI). Linear dichroism in NEXAFS spectroscopy reveals that DPNDI adopts a standing-up configuration on Zn- and Co-TPP as a result of nitrogen–metal axial coordination, whereas it lies flat on the substrate in the case of Cu-TPP. Calculations for a model pyridine ligand indicate stronger binding to Zn and Co centers, assisted by a surface trans effect, while the weaker Cu–pyridine interaction is overcome by the strong DPNDI–TiO_2 interaction. The homeotropic alignment of the ditopic DPNDI ligand on Zn- and Co-TPP exposes coordination sites suitable for the growth of laterally coherent three-dimensional hetero-organic architectures.

440	**Unidirectional Motion of Single Molecules**	Grant Simpson	Contributed talk (17:30-17:45)

Leonhard Grill (1) Mats Persson (2) Grant Simpson (1)

(1) University of Graz
(2) University of Liverpool

The purpose of a molecular motor is to convert external energy into unidirectional motion. Feringa-type molecular motors, in which double-bond isomerisation leads to large geometric changes in the molecule, are known to undergo rapid unidirectional motion in solution but often have a reduced function when adsorbed on a surface. In contrast, recently discovered adsorbate motors [1] do not exhibit large structural changes and thus their motion is efficient and unidirectional when adsorbed on a metal surface. Using a scanning tunnelling microscope (STM), we track such motion at the single-molecule scale. The motion is triggered by an internal proton transfer reaction. We further show that, by altering the local chemical structure, this tautomerisation can be affected and may result in modulation of the unidirectional molecular translation.

[1] G. J. Simpson, M. Persson, L. Grill, Nature, 621, 82-86 (2023)

86	**On-Surface Coupling of Feringa-Type Molecular Motors**	David Le	Contributed talk (17:45-18:00)

David Le (1) Grant J. Simpson (1) Matthew J. Timm (1) Christophe Nacci (1) Dongdong Liu (2) James M. Tour (2) Leonhard Grill (1)

(1) University of Graz
(2) Rice University

Artificial molecular motors are fundamental components of nanoscale machines that convert external energy into uni-directional motion. On metallic surfaces, their operation can be probed with sub-molecular precision, allowing observation of rotational pathways and intermediates.
In nanomachines, it could be advantageous to have not only one, but several motor units incorporated. However, the synthesis of such complex molecules is very challenging. Here, we studied whether individual Feringa-type motor units can be coupled covalently directly on a Au(111) surface to form bimotors, thus avoiding the complex synthesis and difficult deposition of molecules that contain more than one motor unit. Using low-temperature scanning tunnelling microscopy (STM) under ultrahigh vacuum conditions, we identified individual bimotor molecules after the coupling and could resolve distinct conformations. Moreover, conformational transitions and lateral translation could be induced by STM tip manipulation. In addition to discrete bimotor formation, we also observed chain growth of molecular motors on Au(111) from a different monomotor precursor.
Our results demonstrate controlled reactions and manipulation of molecular motors on a metallic surface, supporting the development of more complex nanomachines.

OGD – Session 2 (Wed 23, 16:00-18:00)

ID	Title	Speaker	Type
747	**Atomic-Scale Optical Microscopy with Continuous-Wave Mid-Infrared Light**	Yaroslav Gerasimenko	Contributed talk (16:00-16:15)

Yaroslav Gerasimenko (1) Felix Schiegl (2) Valentin Bergbauer (2) Svenja Nerreter (2) Valentin Giessibl (2) Franz J. Giessibl (2) Tom Siday (3) Markus Huber (2) Rupert Huber (2)

(1) University of Graz
(2) Universität Regensburg
(3) University of Birmingham

Recent discoveries of correlated phases in two-dimensional quantum materials have created a strong demand for optical techniques capable of resolving electronic and structural features at the atomic scale. Near-field microscopy (SNOM) breaks the diffraction limit by coupling light to a sharp metallic tip, but achieving the atomic-scale optical resolution remains a formidable challenge. Recent advances in lightwave-driven scanning tunneling microscopy have opened a new route: intense terahertz and mid-infrared fields can drive tunneling currents through an atomically confined junction. However, detecting the associated optical emission in a SNOM-style readout remains challenging because the emitting volume is extremely small. Here, we show that even continuous-wave MIR radiation from a commercial quantum cascade laser can induce tunneling currents strong enough for direct optical detection [1]. Using picometer-stable qPlus-based tip-sample control under UHV and cryogenic conditions, we detect a strongly localized optical response near an Au(111) surface, marked by a rapid increase in scattered amplitude and a pronounced optical phase shift at tunneling distances. Lateral scans across monoatomic gold steps reveal optical contrast confined to the ångström scale and closely correlated with the simultaneously measured tunneling current. These signatures closely resemble recent pulsed-THz results, where radiation was emitted from AC tunneling currents driven by optical near fields, enabling all-optical subcycle microscopy on atomic length scales [2]. Together, these results establish continuous-wave near-field optical tunneling emission as a practical route toward atomic-scale optical microscopy with widely accessible tabletop light sources.

[1] F. Schiegl et al., Nano Letters 26, 1689–1696 (2026)
[2] T. Siday et al., Nature 629, 329–334 (2024)

581	**Online Monitoring of the Oxygen Adsorption on Cu(110) with PEEM and DRS**	Robert Heller	Contributed talk (16:15-16:30)

Robert Heller (1) Peter Zeppenfeld (1) Thorsten Wagner (1)

(1) JKU, Institute of Experimental Physics, Surface Science Division

We studied the dissociative adsorption of oxygen on the Cu(110) surface using Photoelectron Emission Microscopy (PEEM) and Differential Reflection Spectroscopy (DRS) simultaneously. Unlike many experiments carried out already in the 1970s and 1980s, our approach focusses on real-time monitoring. For oxygen exposures up to ~100L, at temperatures between 350K and 420K, the process saturates at an oxygen coverage of 0.5 with a well-ordered (2×1)O superstructure. At intermediate coverages, a regular pattern of alternating Cu and CuO stripes is formed [1]. We used a PEEM with a xenon lamp (Xe) to study changes in the electron yield (EY) during the exposure. Oxygen adsorption causes a decrease in EY and, hence, an increase in the work function. Since our DRS setup uses the same light source as the PEEM, we can synchronously record the change of the reflectance and reliably compare the two signals. Interestingly, the normalised adsorption curves are not identical, indicating that the PEEM and/or the DRS signals are not directly proportional to the oxygen coverage. This could be related to the effect of the formation of the nanostructured Cu-CuO stripe pattern upon oxygen adsorption [1].

[1] K. Kern et al., Phys. Rev. Lett. 67, 855 (1991).

735	**Thermal Activation of CO_2 on Fe_2O_3(012)**	Johannes Filzmoser	Contributed talk (16:30-16:45)

Johannes Filzmoser (1) Moritz Eder (1) Florian Kraushofer (1) Jiri Pavelec (1) Gareth Parkinson (1)

(1) TU Wien

The adsorption of CO_2 on hematite α-Fe_2O_3(012) was investigated in ultra-high vacuum (UHV) using temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS). CO_2 adsorption on this surface exhibits unusual behavior in TPD for coverages up to one molecule per unit cell (corresponding to 0.5 molecules per Fe^{2+} cation). Two desorption features centered around 150 K, and 220 K increase concurrently with increasing coverage. IRAS measurements reveal that this behavior arises from the thermal activation of weakly bound, physisorbed CO_2 at temperatures above 100 K. Infrared bands in the carbonate region appear, indicating that activated CO_2 interacts with surface oxygen to form surface carbonate (CO_3^{2-}) species. This activation

pathway directly competes with molecular desorption. By supplying CO_2 at temperatures just below the carbonate desorption temperature, enhanced surface carbonate coverages can be achieved. These findings contribute to our understanding of CO_2 activation on Fe_2O_3 (012) and will be a prerequisite for surface reaction studies.

661	**Environmental Stability of Model Single-Atom Catalysts**	Florian Kraushofer	Contributed talk (16:45-17:00)

Florian Kraushofer (1) Alexander Syböck (1) Lena Haager (1) Panukorn Sombut (1) Ali Rafsanjani-Abbasi (1) Florian Buchner (1) Faith J. Lewis (1) Moritz Maximilian Joachim Eder (1) Jiří Pavelec (1) Erik Rheinfrank (1) Giada Franceschi (1) Michele Riva (1) Matthias Meier (2) Cesare Franchini (2) Michael Schmid (1) Ulrike Diebold (1) Georg K. H. Madsen (1) Gareth S. Parkinson (1)

(1) TU Wien
(2) University of Vienna

Single-Atom Catalysis (SAC) may provide unique reactivity and ideal dispersion of the active metal. However, while many examples have been synthesized successfully, there is a fundamental mismatch between most experimental work and the theoretical modelling of these systems. Applied catalysts are based on complex powder supports, and are fabricated and used in environments containing various potential ligands and contaminants. In contrast, theoretical treatment is generally based on density functional theory (DFT) calculations assuming low-index facets on idealized supports, often placing the single catalyst atom in a bulk-continuation site. Single-crystal supports prepared in UHV provide a direct experimental analogue to DFT and a bridge to more complex systems, validating or correcting the sites assumed by theory.
We have developed two SAC model systems on iron oxides single crystals, the (001) facet of magnetite (Fe_3O_4) and the $(1\bar{1}02)$ facet of hematite (α-Fe_2O_3).[1,2] UHV-based experiments have shown that simple ligands such as CO and H_2O, which will be present in most realistic conditions, can both stabilize or destabilize the metal adatoms: If the pristine, UHV-prepared surface already presents a good binding template, as is the case on Fe_3O_4 (001), added ligands may weaken the catalyst–support interaction, thus inducing mobility and agglomeration.[3,4] On the other hand, when ligands bind to both adatoms and support, they can stabilize the single-atom configuration and prevent clustering, as is the case with water on α-$Fe_2O_3(1\bar{1}02)$.[5] I will show how these ligand-mediated stabilization and destabilization mechanisms translate to more realistic environments, i.e., liquid and (near-)ambient pressure environments of H_2O, O_2, and CO.

1. R. Bliem et al., Science 2014, 346, 1215
2. F. Kraushofer et al., J. Phys. Chem. C 2018, 122, 1657
3. G. S. Parkinson et al., Nat. Mater. 2013, 12, 724
4. R. Bliem et al., Proc. Natl. Acad. Sci. 2016, 113, 8921
5. F. Kraushofer et al., ACS Energy Lett. 2022, 7, 375

716	**Hydrogen Activation via Dihydride Formation on a $Rh_1/Fe_3O_4(001)$ Single-Atom Catalyst**	Gareth Parkinson	Contributed talk (17:00-17:15)

Gareth Parkinson (1) Nail Barama (1) Ulrike Diebold (1) Cesare Franchini (2) Maosheng Hao (1) Florian Kraushofer (1) Florian Libisch (3) Matthias Meier (2) Jiri Pavelec (1) Lena Puntscher (1) Michael Schmid (1) Panukorn Sombut (1) Chunlei Wang (1)

(1) Institute of Applied Physics, TU Wien, Austria
(2) Computational Materials Physics, University of Vienna, Austria
(3) Institute for Theoretical Physics, TU Wien, Austria

Hydrogen activation is a key elementary step in catalytic hydrogenation. In heterogeneous catalysis, it usually proceeds through dissociative adsorption on metal nanoparticles followed by surface diffusion or spillover, whereas homogeneous catalysts activate H2 through dihydride or dihydrogen intermediates at a single metal center. Here, we show that isolated Rh adatoms supported on Fe3O4(001) activate hydrogen through formation of a stable dihydride species without atomic H spillover. Temperature-programmed desorption, x-ray photoelectron spectroscopy, and scanning tunneling microscopy collectively reveal strong (≈1 eV) hydrogen adsorption exclusively at isolated Rh1 sites, while isotope-exchange experiments further demonstrate that hydrogen remains localized. Density-functional theory-based calculations indicate a barrierless conversion from molecular H2 to the dihydride, and random-phase approximation calculations further confirm the relative stability of the dihydride. Together, these results show that single-atom Rh sites cleave hydrogen through a dihydride pathway analogous to homogeneous complexes, establishing a mechanistic bridge between homogeneous and heterogeneous catalysis.

365	**Simplifying Surface Structure Search by LEED *I(V)***	Michael Schmid	Contributed talk (17:15-17:30)

Alexandra M. Imre (1) Florian Kraushofer (1) Michele Riva (1) Paul Haidegger (2) Ulrike Diebold (1) Lutz Hammer (3) Michael Schmid (1)

(1) Institute of Applied Physics, TU Wien, Austria
(2) Institute of Applied Physics and Research Unit of Databases and Artificial Intelligence, TU Wien, Austria
(3) Solid State Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Quantitative low-energy electron diffraction [LEED $I(V)$] is a powerful method for surface-structure determination, based on the comparison of experimentally observed diffraction intensities I with computations for structural models. As the diffraction intensities are highly sensitive to subtle structural changes, local structure optimization is essential for assessing the validity of a structure model and finding the best-fit structure. The ViPErLEED project (Vienna Package for Erlangen LEED) drastically reduces the user effort required for LEED $I(V)$ studies [1,2]. The talk will focus on two recent developments. A new implementation of structure search reformulates the optimization problem in a way that allows the use of standard optimization algorithms, including gradient-based methods [3]. This new code is based on JAX and can make use of graphics processing units (GPUs), accelerating structure search by more than an order of magnitude. Structure optimization requires a measure of agreement between the calculated and experimental data, a so-called R factor. We show that the previously used R factor R_P (introduced by J. Pendry) has several deficiencies and is ill-suited for gradient-based optimization. We present an improved R factor R_S that avoids these problems and is as good as or better in steering the optimization to the correct result [4]. As an example for the application of these new developments, a new structure model of the $Fe_2O_3(1\bar{1}02)$-(2×1) surface will be presented.

[1] Kraushofer et al., Phys. Rev. Res. 7, 013005 (2025)
[2] Schmid et al., Phys. Rev. Res. 7, 013006 (2025)
[3] Imre et al., arXiv:2512.09737
[4] Imre et al., J. Phys.: Condens. Matter 38, 105001 (2026)

448	**Nonadiabatic Energy Loss in Hyperthermal Gas-Surface Scattering: Going Beyond the Mean Field Approximation**	Ash Baldwin	Contributed talk (17:30-17:45)

Ash Baldwin (1) Reinhard Maurer (1,2)

(1) University of Vienna
(2) University of Göttingen

Nonadiabatic energy dissipation is known to play a crucial role in hyperthermal scattering at surfaces, leading to electron-hole pair excitation and highly inelastic scattering. For projectiles with unpaired spins, such as hydrogen atoms, hybridisation with the metal surface results in strong non-adiabatic effects driven by a phase transition in its spin-polarisation. It is known that traditional mean-field descriptions of the resultant nonadiabatic dynamics using methods like MDEF and Ehrenfest dynamics break down in the presence of the transition, leading to divergent energy transfer rates and unphysical stopping powers at the location of the spin transition [Box et al. J. Phys. Chem. Lett. 15, 51 (2024); Lindenblatt et al. Phys. Rev. Lett. 97 (2006)].
Here, we model H/Cu(111) and H/Ag(111) scattering in the presence of on-site correlation in the adsorbate state using the Newns-Anderson Hamiltonian. We go beyond previous works by simulating the dynamics using stochastic trajectory surface hopping methods that capture the coupling between the nuclear and electronic degrees of freedom beyond the mean-field. We systematically classify scattering regimes and assess the applicability of mean-field and beyond mean-field methods for predicting the nonadiabatic energy loss in these regimes.

449	**Interface Engineering by ALD–PVD Supercycles: Materials-by-Design Strategy for Photo(electro)catalysis**	Alberto Perrotta	Contributed talk (17:45-18:00)

Regina Del Sole (1) Simelys Hernandez (2) Carlo Pastore (3) Antonella Milella (1) Alberto Perrotta (1) Sara Lotito (4) Sofia Belen Cosseddu (2) Paolo Martorelli (2) Hilmar Guzmán (2) Fabio Palumbo (5) Francesco Fracassi (1)

(1) Università degli Studi di Bari
(2) Politecnico di Torino, Department of Applied Science and Technology (DISAT), CREST Group, Torino, Italy
(3) CNR-IRSA
(4) Luxembourg Institute of Science and Technology (LIST)
(5) CNR-NANOTEC

Controlling interfacial charge transfer is vital for designing thin-film materials for CO_2 electroreduction (eCO_2RR) and photocatalytic H_2 production. We employ atomic layer deposition (ALD)–physical vapor deposition (PVD) supercycles to engineer ZnO/Cu interfaces with sub-nanometer precision. XPS and EDX analysis confirm sub-at.% Cu incorporation and strong electronic coupling, enabling precise modulation of interface density and defect states while maintaining conformality on porous substrates.
In eCO_2RR, ZnO/Cu-modified GDEs achieve current densities of 100 mA cm^{-2} and Faradaic efficiencies for CO up to 72% at 20 mA cm^{-2}, with CO_2 conversion exceeding 30%. Operando restructuring, evidenced by morphological reconstruction and surface composition shifts, does not lead to immediate failure, with optimized energetics allowing operation below 2.5 V, enabling direct photovoltaic-to-fuel integration.
In photocatalytic H_2 generation, ALD-grown ZnO films significantly outperform commercial powders, reaching up to 1000 µmol g^{-1}. A critical design rule is established: surface-only Cu yields ~832 µmol g^{-1}, whereas embedding Cu within the ZnO matrix increases productivity to 5660 µmol g^{-1} (>5× vs. pristine ZnO). This demonstrates that subsurface (buried) junctions are decisive for promoting charge separation and suppressing recombination.
Ultimately, functionality in both platforms emerges from the interplay of interface density, band alignment, and defect-mediated transport. These results establish ALD–PVD supercycles as a robust materials-by-design strategy for tailoring interfacial properties, offering clear guidelines for designing high-performance oxide/metal catalysts.

OGD – Session 3 (Thu 24, 16:00-18:00)

ID	Title	Speaker	Type
295	**Manipulation of Atomically Precise Nanostructures from Single Atoms and Molecules**	Nikita G. Osipov	Contributed talk (16:00-16:15)

Nikita G. Osipov (1) Christophe Nacci (1) Grant J. Simpson (1) Leonhard Grill (1)

(1) Institute of Chemistry, University of Graz, Austria

Quantum corrals are of particular interest in surface science as they can be used to investigate quantum phenomena, such as quantum mirage (1) or function as quantum simulators that mirror the electronic properties of real atoms or molecules (2).
Currently, investigating these prominent structures requires researchers to manually assemble the objects on a surface using atomic manipulation techniques, a process that is extremely time-consuming. Our work aims to solve this critical bottleneck and save valuable research time.
A primary goal of our project is to create an instrument for automatic and autonomous atomic manipulation. We are developing this system using machine learning algorithms to enable the careful, precise positioning of atoms or molecules (3). This novel instrument will facilitate the assembly of large-scale objects or complex compositions of multiple smaller ones with high precision, thereby enabling the collection of significantly more data.
In this work, we our current status of assembled quantum corrals on noble metal surfaces. First results of manually assembled nanostructures will be presented together with the computational algorithm in the automated construction.

(1) Li, Q., Li, X., Miao, B. et al. Kondo-free mirages in elliptical quantum corrals. Nat Commun 11, 1400 (2020)
(2) E. Sierda et al., Quantum simulator to emulate lower-dimensional molecular structure. Science 380, 1048-1052 (2023)
(3) B. Ramsauer, G. J. Simpson, J. J. Cartus, A. Jeindl, V. García-López, J. M. Tour, L. Grill and O. T. Hofmann, Autonomous single-molecule manipulation based on reinforcement learning, Journal of Physical Chemistry A 127, 2041 (2023)

616	**Correlation-Driven d-Band Modifications Promote Chemical Bonding at 3d-Ferromagnetic Surfaces**	Giovanni Zamborlini	Contributed talk (16:15-16:30)

Giovanni Zamborlini (1)

(1) University of Graz, Institute of Physics

Accessing the interfacial electronic structure of ferromagnets (FM) with spin and momentum resolution is crucial for predicting the electronic functionality of hybrid interfaces. In particular, the adsorption of non-magnetic atoms or molecules on a ferromagnetic transition-metal surface creates complex hybrid systems exhibiting a variety of different physical phenomena.
First, I will describe how oxygen adsorption strongly modifies the electronic properties of the pristine Fe(100) surface (O–Fe), enhancing electronic correlations [1]. The spin-dependent electronic structure is accessed by spin-resolved photoemission electron microscopy, combined with advanced theoretical approaches that explicitly account for electron correlation effects.
This oxygen-passivated surface provides a versatile platform for molecular adsorption. In particular, we investigate pentacene adsorption on O–Fe(100), where the enhanced electron correlation at the surface promotes strong molecule–metal interaction. A combination of photoemission orbital tomography (POT), scanning tunneling spectroscopy (STS), and electronic structure calculations reveals pronounced hybridization between the pentacene frontier orbitals and the Fe 3d states. A tailored DFT+U approach with a negative effective on-site interaction (Ueff = −3.1 eV) reproduces the experimentally observed reduction in d-band spin splitting and band narrowing, consistent with dynamical mean-field theory. These correlation-induced modifications enhance the energetic overlap between metal d-states and molecular orbitals, driving a transition from physisorption to strong chemisorption [2].

[1] D. M. Janas et. al. Advanced Materials 2023, 35, 2205698.
[2] D. M. Janas et. al. Small 2025, 22, e08952

654	**Exploring Correlation-Driven Adsorption on Oxygen-Passivated Fe(001) with DFT+U**	Andreas Windischbacher	Contributed talk (16:30-16:45)

David Janas (1) Andreas Windischbacher (2) Mirko Cinchetti (1) P. Puschnig (2) Giovanni Zamborlini (1)

(1) Department of Physics, TU Dortmund University
(2) Institute of Physics, University of Graz, 8010 Graz, Austria

The role of many-body effects at adsorbate-metal interfaces is a crucial – but often overlooked – factor in designing materials for spintronic and electrocatalytic applications. Correlation-driven modifications to the electronic structure of ferromagnetic surfaces can promote surface-adlayer interactions and enhance surface reactivity [1,2]. A prime example is the oxygen-passivated Fe(100) surface, where a chemisorbed layer of oxygen leads to spin-dependent band broadening, narrowing of Fe d-bands near the Fermi energy, and a reduction in the exchange splitting [3].
Modelling the influence of these modifications on adsorbates is a theoretical challenge. Such systems are usually poorly described by standard density functional theory (DFT), while the size of the unit cell currently renders more advanced approaches like dynamical mean-field theory computationally prohibitive. Interestingly, we found that a tailored DFT+U approach with a negative effective on-site interaction (U_{eff} = −3.1 eV) captures the experimentally observed electronic structure surprisingly well. In specific, we present the analysis of three different system, namely Fe-O covered with a monolayer of MgO, Pentacene, and fluorinated TCNQ. We show that the unconventional use of DFT+U is able to reproduce important interface properties, such as the energetic overlap between metal d-states and adlayer orbitals, which governs the transition between physisorption and chemisorption. Our theoretical findings are confirmed by momentum-resolved photoemission orbital tomography and scanning tunnelling spectroscopy data.

[1] Cao, A. and Nørskov, J.K.. ACS Catal., 2023, 13, 3456.
[2] Zhang, K., et al. Science, 2024, 383, 1357.
[3] Janas, D.M., et al. Adv. Mater., 2023, 35, 2205698.

426	**Adsorption-Induced Modification of the Surface Resonant Vibrational Response on Cu(110)**	Sarang Bhasme	Contributed talk (16:45-17:00)

Sarang Bhasme (1) Mariella Denk (1) Mohamed Yassine Fatihi (2) Simone Sanna (2) Peter Zeppenfeld (1)

(1) Surface Science Division, Institute of Experimental Physics, Johannes Kepler University
(2) Institut für Theoretische Physik and Center for Materials Research (LaMa), Justus-Liebig-Universität Gießen

Surface Resonant Raman Scattering (SRRS) is used to probe surface phonons of Cu(110) via resonant coupling to surface electronic states [1]. In combination with Reflectance Difference Spectroscopy (RDS), we investigate adsorption-induced modification of the vibrational response under ultra-high vacuum conditions. Time resolved measurements during controlled CO and O_2 exposure reveal systematic changes in surface phonon-related features, indicating a modification of the surface electronic resonance condition upon adsorption. Based on this sensitivity, we extend SRRS to molecular adsorbates. First test measurements on Dihydrotetraazapentacene (DHTAP) on Cu(110) demonstrate the feasibility of detecting molecular vibrational signals under resonant conditions. These results establish SRRS as a sensitive probe of adsorption-induced changes on metal surfaces and provide a route towards studying more complex molecule-surface systems.

[1] M. Denk et al., Phys. Rev. Lett. 128, 216101 (2022).

243	**Excited State Population Transfer Dynamics in Squaraine Microtextured Thin Films Investigated with Femtosecond Transient Absorption**	Patricia Magdalena Brugger	Contributed talk (17:00-17:15)

Patricia Magdalena Brugger (1) Jakub Dóstal (2) Andrej Hovan (2) Markus Koch (1) Arne Lützen (3) Peter Puschnig (4) Manuela Schiek (5) Marvin F. Schumacher (3) Robert Schwarzl (1) Narges Taghizade (4) Andreas Windischbacher (4) Niko Zöch (1)

(1) TU Graz
(2) ELI beamlines ERIC
(3) University of Bonn
(4) University of Graz
(5) Johannes Kepler University, Linz

Squaraine dyes are a unique class of organic semiconductors, featuring properties such as strong absorption in the visible and near infrared, high photostability and low biotoxicity, resulting in a range of applications reaching from photovoltaics to biomedical applications. Here, we focus on 2,4-bis[4-

(N,N-diisobutylamino)-2,6-dihydroxyphenyl]squaraine (SQIB), which exhibits an orthorhombic crystal structure, containing four molecules per unit cell. Davydov splitting into four sublevels is induced by Coulombic interactions, with three of them being optically active while the fourth is a dark state, due to a vanishing transition dipole moment from the ground state. The population transfer dynamics between the Davydov components, including the dark state, determine the energy- and charge-transfer dynamics of SQIB but have evaded observation so far.[1]
To go past the steady-state optical properties we performed transient absorption microscopy with a temporal resolution on the femtosecond scale.[2] We observed several excited state absorption (ESA) features as well as the subsequent population transfer and vibrational cooling. Moreover, the temporal evolution of some of the spectral features indicates the involvement of the dark state in the population dynamics. Additional calculations based on the Bethe-Salpeter equation (BSE), provided by our cooperation partners, as well as recent publications using the Frenkel-Holstein Hamiltonian, are taken into account for the interpretation of our measurements.

[1] D. Giavazzi, R. Schwarzl, M. Koch, M. Schiek, A. Painelli, F. Spano, J. Phys. Chem. Lett. 16, 41, 10763–10770 (2025)
[2] R. Schwarzl, P. Heim, M. Schiek, D. Grimaldi, A. Hohenau, J. Krenn, M. Koch, Opt. Express 30, 34385-34395 (2022)

663	**Orientation Control in MOF Thin Films: Spin-Assisted LbL-LPE Growth probed by GIWAXS**	Eleonora Afanasenko	Contributed talk (17:15-17:30)

Eleonora Afanasenko (1) Heinz Amenitsch (2) Sumea Klokic (2) Benedetta Marmiroli (2)

(1) CERIC-ERIC
(2) Institute of Inorganic Chemistry, Graz University of Technology

Precise control over crystallographic orientation in metal–organic framework (MOF) thin films is essential for harnessing their functional properties, including anisotropic transport, guest diffusion and flexibility. Aligning the MOF lattice along a defined crystallographic direction enables enhanced, directional performance in applications such as sensing, catalysis, and molecular separation. In this study, we present a fabrication method for the controlled growth of (001)- and (100)-oriented thin films of the model system Zn_2BDC_2DABCO (BDC = terephthalate; DABCO = 1,4-diazabicyclo[2.2.2]octane).
Our spin-assisted layer-by-layer liquid-phase epitaxy (LbL-LPE) approach selectively yields amorphous films, face-on (001)-oriented films, or nearly edge-on (100)-oriented structures by tuning the synthesis conditions [1]. The effectiveness and reproducibility of the method are confirmed by quantitative analysis of synchrotron GIWAXS data across multiple samples, using the degree of orientation (DO) and the Hermans orientation parameter (HOP) extracted from the azimuthal intensity distribution of the (001) reflection. Mapping DO and HOP as a function of synthesis conditions, number of growth cycles, and different interface chemistry (16-mercaptohexadecanoic acid or (4-(4-pyridyl)phenyl)methanethiol self-assembled monolayer) allowed us to identify fabrication regime that supports near-single-crystal growth.
Beyond this system, the proposed analysis offers a streamlined GIWAXS workflow for evaluating qz reflections when pole figures down to $\gamma = 0°$ are not accessible. This enables reliable comparison between datasets, robust assessment of synthesis reproducibility, and direct extension to related oriented MOF film systems.

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632	**Deracemization in 1,1'- Binaphthyl Thin Films and Electronic Circular Dichroism**	Sanjay John	Contributed talk (17:30-17:45)

Sanjay John (1) Yves Geerts (2,3) Tiberiu-Marius Gianga (4) Ann Maria James (1) Roland Resel (1) Giuliano Silligardi (4) Oliver Werzer (5)

(1) Institute of Solid State Physics, Graz University of Technology, Austria
(2) Free University of Brussels (ULB)
(3) International Solvay Institutes
(4) B23 Beamline, Diamond Light Source
(5) Joanneum Research MATERIALS

1,1'-binaphthyl is an axially chiral molecule that crystallizes in either racemic phase, consisting of an equal number of both enantiomers in the unit cell or in a chiral phase where only one type of enantiomer is present. Thin film crystallization kinetics are strongly influenced by the presence of a solid substrate, where selective adsorption at the substrate–liquid interface promotes heterogeneous nucleation and complete chiral phase formation. This study further explores the deracemization of 1,1' -binaphthyl through the influence of a chiral additive, 1,1'-bi-2-naphthol. Structural characterization by Grazing Incidence XRD (GIXD) using synchrotron radiation confirms that thin films prepared by solution processing crystallize preferentially in the chiral phase. The extent of deracemization and enantioselectivity is further investigated using electronic circular dichroism (ECD). For the first time, the solid-state ECD spectra of 1,1'-binaphthyl thin films are recorded using conventional ECD spectrometer and synchrotron-based Mueller Matrix Polarimetry (MMP). Since conventional ECD measurements cannot resolve intrinsic ECD from linear anisotropies such as linear dichroism (LD) and birefringence (LB), spatially resolved Mueller matrix polarimetry is employed to accurately extract true solid-state ECD. MMP mapping on the thin film samples reveals localized chiroptical responses within the 1,1'-binaphthyl thin films, providing direct insight into enantioselective crystallization and spatially resolved chiral purity.

526	**Current-Driven Rb^+ Intercalation for On-Chip Tuning of Superconductivity in Rb_xC_{60} Thin Films**	Konstantin P. Shchukin	Contributed talk (17:45-18:00)

Konstantin P. Shchukin (1) Baptiste Coquinot (2) Yannic Falke (3) Oliver Gallego Lacey (4) Alexander Grüneis (1) Jingsong Huang (5) Jacek Jakowski (6) Ram Prakash Pandeya (1) Patrik Staudenmayer (1)

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(2) Institute of Science and Technology Austria (ISTA)
(3) II. Physikalisches Institut, Universität zu Köln
(4) CEA, Universite Grenoble Alpes
(5) Computational Sciences & Engineering Division, Oak Ridge National Laboratory
(6) Center for Nanophase Materials Sciences, Oak Ridge National Laboratory

The synthesis of superconducting fullerides is conventionally performed by intercalation of alkali ions via thermal gradients [1-4] or from solution [5-6]. Both methods have poor stoichiometry control, and thermal intercalation requires sample heating. Here we introduce electro-intercalation to directly drive Rb^+ into C_{60} thin films with high stoichiometric precision. We use a new ultra-high vacuum (UHV) setup that combines \textit{in-situ} film preparation with in-operando Raman spectroscopy and four-terminal electronic transport [7].

The precise stoichiometry of the superconducting Rb_3C_{60} phase is identified by the $A_g(2)$ Raman mode at about 1449 cm^{-1}, clearly distinct from pristine C_{60}. By varying the Rb/C_{60} ratio we show that the intensity ratio of the Rb_3C_{60} and C_{60} Raman peaks correlates with the superconducting transition temperature T_C. We demonstrate on-chip synthesis of superconducting Rb_xC_{60} films and tuning of T from about 7 K up to nearly 26 K when the stoichiometry is adjusted from $Rb_{2.7}C_{60}$ to Rb_3C_{60}. Time-dependent Raman and transport data show that the Rb^+ electro-intercalation follows Butler–Volmer-type kinetics driven by the applied current.
Electro-intercalation thus provides a powerful route for precise, on-chip control of superconductivity in ultra-thin fulleride films and is extendable to other layered and porous materials.

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OGD – Session 4 (Fri 25, 10:30-12:30)

ID	Title	Speaker	Type
625	**Investigating the Kinetics of Porphyrin Self-Metalation on Ultrathin MgO: The Role of Charge Transfer**	Francesco Presel	Contributed talk (10:30-10:45)

Francesco Presel (1) Christian Simon Kern (1) Maximilian Laßhofer (1) Tomáš Skála (2) Georg Koller (1) P. Puschnig (1) Martin Sterrer (1)

(1) Institute of Physics, University of Graz
(2) Charles University Prague

On-surface reactions including self- and trans-metalation of organic molecules on surfaces play a major role in the fields of organic electronics and molecular self-assembly[1]. They can on one hand provide additional pathways, or even the only method, to obtain specific structures, thereby providing a tool to tailor the properties of molecular layers; but on the other hand, unwanted reactions can negatively affect their stability and limit their applications. While such types of reactions have been extensively studied on metal surfaces, it was long believed that they would be hindered on oxides, due top the stronger bonds within such solids. However, in previous experiments, we have shown that porphyrins, which represent a versatile class of organic molecules, can self-metalate when adsorbed on ultrathin magnesium oxide film[2].
On such surface, self-metallation is not the only chemical process occurring: charge transfer can also be observed, depending on the difference between the electron affinity of the adsorbate and the surface work function[3], with either process having been observed regardless of the other[4].
Here we show that the interplay between these two processes is much more subtle, with the charge state of the molecule affecting primarily the adsorption geometry and thereby also the energy barriers for the self-metallation of porphyrins of different size. Temperature-resolved XPS measurements, combined with DFT calculations, reveal that charge transfer actually increases the barrier for self-metallation reactions, thereby stabilising the structure at least up to room temperature. These results provide fundamental understanding to the parameters which must be tuned to fully control on-surface reactions on oxide surfaces and thin films.

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[3] Hurdax et al., Adv. Mater. Interf., 2020, 7, 2000592
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ID	Title	Speaker	Type
157	**In situ Characterization of Nanoporous Copper Evolution during Electrochemical Dealloying**	Samuel Graf	Contributed talk (10:45-11:00)

Samuel Graf (1) Mislav Sušac (1) Bernd Nidetzky (1) Roland Würschum (1)

(1) Graz University of Technology

Nanoporous metallic structures are of interest for sensing and catalysis applications due to the large internal surface area. By starting out with an alloy consisting of elements with different corrosion potentials, electrochemical dealloying can be used to selectively remove the less noble species from the initial alloy. Surface rearrangement of the more noble species then leads to the formation of a self-standing, continuous, nanoporous metallic structure [1]. Research efforts so far have been focused on nanoporous structures produced from gold alloys [2], but for large-scale applications a more cost-effective alternative would be beneficial.
For this purpose, the present work is devoted to nanoporous copper which recently has gained interest as alternative to nanoporous gold. The formation of the nanoporous copper structure during dealloying is comprehensively investigated in-situ by means of chronoamperometry, 4-point resistometry [3], and electrochemical impedance spectroscopy as well as ex-situ by electrochemical and optical characterization [4]. In contrast to nanoporous gold, the porosity evolution and subsequent surface modification of nanoporous copper appears to be hindered by surface oxide formation [5]. However, the insulating oxide could prove beneficial. Therefore, potentials are explored to use nanoporous copper as an alternative carrier structure for the typical gold-based metal-enzyme hybrid electrodes [6,7].

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378	**Machine-Learning Potentials for Nano-Mechanical Simulations of Defective Ceramics: A Case Study of Transition Metal Diborides**	Chunhui Du	Contributed talk (11:00-11:15)

Chunhui Du (1) Nikola Koutná (1) Shuyao Lin (1) Paul Mayrhofer (1) Davide Sangiovanni (2)

(1) TU Wien
(2) Linköping University

Transition metal diborides (TMB_2s) ceramics are highly attractive for protective coating applications due to their high hardness with excellent thermal and chemical stability. Synthesis conditions cause these materials commonly grown as largely off-stoichiometric, consequently, including vacancies or other simple crystallographic defects that alter the intrinsic response to mechanical strains. Therefore, it is now critical to establish an atomic-level understanding of how such defects control the mechanical properties of TMB_2s ceramics.
In this work, molecular dynamics (MD) simulations equipped with here-trained machine-learning interatomic potentials (MLIP) are carried out, to reveal effects of point and planar defects during typical mechanical loading of several paradigm diborides (TMB_2, M = Ti, Ta and W). MLIP training routine consists of active learning on configurations from 0K DFT calculations and finite temperature ab initio molecular dynamics, including equilibrium structures of different phases (α, P6/mmm and ω, $P6_3/mmc$), uniaxial/shear loading states, as well as various defective and/or extremely strained environments. The MLIP's robustness to highly strained environments, particularly near indenter tips, is achieved via on-the-fly training on extrapolative atomistic clusters from simple nanoindentation runs.
Following MLIP's validation, we simulate room-temperature tensile tests and nanoindentation of TMB_2 and $TMB_{2\pm x}$ structures, where TM/B sub-stoichiommetry is realized by disordered TM/B vacancies and planar defects previously observed by electron microscopy.
The results demonstrate that our trained MLIP remain robust throughout all simulations. It also accurately captured phase transformations under various loading conditions. A particularly surprising and non-intuitive prediction is that some non-stoichiometric $TMB_{2\pm x}$ structures with specific defect types can exhibit even higher hardness and Young's modulus comparable to the stoichiometric TMB_2, challenging traditional assumptions about weakening effects of sub-stoichiometry. Moreover, this study elucidates the correlation between formation energies and mechanical responses of these non-stoichiometric structures. Overall, these findings offer valuable insights for advanced defect engineering strategies in the future development of transition metal diboride (TMB_x) thin films.

614	**An Ultra-Thin Body SiGeSn Transistor for Cryogenic Electronics**	Paul Krajiczek	Contributed talk (11:15-11:30)

Paul Krajiczek (1) Johannes Aberl (2) Moritz Brehm (2) Andreas Fuchsberger (1) Nikolas Knaller (1) Daniele Nazzari (1) Enrique Prado Navarette (2) Peter Schweizer (3) Masiar Sistani (1) Lilian Vogl (Max 3) Walter Weber (1) Lukas Wind (1)

(1) Institute of Solid State Electronics, TU Wien, Vienna, Austria
(2) Institute of Semiconductor and Solid State Physics, JKU Linz, Linz, Austria
(3) Max Planck Institute for Sustainable Materials, Düsseldorf, Germany

Transistors capable of operating at cryogenic temperatures are key components for the fast and energy-efficient control and readout circuits of qubit systems. However, the ultra-low power requirements and performance metrics are not met by conventional complementary metal-oxide-semiconductor technology, which has been optimized for room-temperature operation. Here, we propose Si-based Schottky junction field-effect transistors enhanced with ultra-thin SiGeSn layers to address these issues. By combining single-elementary Al contacts to avoid dopant freeze-out and using a multi-gate transistor architecture to suppress reverse junction leakage current, a fivefold increase in on-current and a threefold increase in peak transconductance were achieved compared to a Si reference device. Importantly, the presented SiGeSn SBFET delivers on-currents comparable to those of state-of-the-art GeSn transistors, while providing a better on/off ratio. Measurements down to 4.5 K revealed a drain current modulation over nine orders of magnitude with improved inverse subthreshold slopes of 20 mV/dec below 50 K and 50\% reduced threshold voltages, while the on-currents remain mostly temperature-independent, making the system interesting for cryogenic computing. To verify the capabilities of the proposed SiGeSn transistor for cryogenic electronics, a fundamental common-source amplifier circuit was investigated.

565	**Contact Forces in Microgel Suspensions**	Fran Ivan Vrban	Contributed talk (11:30-11:45)

Fran Ivan Vrban (1) Primoz Ziherl (1,2) Antonio Šiber (3)

(1) Facutly of Mathematics and Physics, University of Ljubljana
(2) Jozef Stefan Institute
(3) Institute of Physics, Zagreb, Croatia

Within a model where micrometer-size soft colloidal particles are viewed as liquid drops, we theoretically study the contact interaction between them. We compute the exact deformation energy across a broad range of indentations and for various model parameters, and we show that it can be reproduced using truncated superball and spheropolyhedral variational shapes in the attractive and the repulsive regime, respectively. At large surface tensions representative of microgels, this energy is pairwise additive well beyond small indentations and can be approximated by a power-law dependence on indentation with an exponent around 2.

535	**Mesoscopic Simulations of Thin liquid Films: A Lattice Boltzmann Approach to Wetting and Fluctuations**	Stefan Reimann-Zitz	Contributed talk (11:45-12:00)

Stefan Reimann-Zitz (1)

(1) Research Center Pharmaceutical Engineering, Graz

We present an efficient numerical framework for the simulation of thin-liquid-film hydrodynamics, implemented via the lattice Boltzmann method (LBM) [1]. By adapting models originally developed for shallow-water equations, our method recovers the governing lubrication equations in the long-wavelength and low Reynolds number limits. This approach bridges the gap between molecular-scale interactions and macroscopic hydrodynamic flows, leveraging the inherent parallelism of the LB method to provide high-performance computing capabilities on both CPUs and GPUs.
The reliability of the method is established through theoretically verified use cases. Validation tests demonstrate that the scheme correctly captures the various thin film phenomena. Furthermore, the model accurately simulates the dynamics of droplets and rivulets on complex substrates.
We further showcase the method's versatility by incorporating thermal fluctuations and time-dependent wettability. By equipping the solver with a stochastic term, we accurately capture the impact of thermal noise on film rupture, showing that fluctuations consistently accelerate dewetting across various contact

angles [2,3]. Additionally, we explore the stability of ring-rivulets on substrates with evolving wettability profiles. We demonstrate how tuning substrate heterogeneity allows for precise control over the breakup into discrete droplets, a feature critical for microfluidic applications. This framework provides a robust tool for studying industrial and biological coating processes, offering a scalable solution for complex, multi-scale wetting phenomena [4].

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OGD – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
759 **P099**	**Microscopic and Spectroscopic Study of Pt and Ni Clusters on Pd(100)-Supported MoO_3 Model Thin Films**	Karl Glaser	Poster

Karl Glaser (1) Melissa Stifter (1) Falko Netzer (1) Martin Sterrer (1) Svetlozar Surnev (1)

(1) University of Graz, Institute of Physics

Molybdenum trioxide (MoO_3) is an industrially important semiconducting material, widely used in applications such as catalysis, rechargeable batteries and gas sensors. A key advantage of MoO_3 is the flexibility of the Mo oxidation state, which can be easily tuned. In this presentation, we will discuss the applicability of model MoO_3 single-crystalline thin films as supports for metal atoms and clusters, specifically, Pt and Ni. We present our latest results on the adsorption of Pt and Ni on various MoO_3 thin films, namely the c(2x2)-MoO_3 monolayer (ML), the reduced (3x3)-Mo_5O_8 ML, the MoO_3-bilayer (BL), and the MoO_{3-x}-trilayer (Magnéli phase). These films were prepared in UHV by physical vapor deposition (PVD) on a Pd(100) single crystal and further investigated by Low Energy Electron Diffraction (LEED), Scanning-Tunneling Microscopy (STM), X-Ray Photoelectron Sepctroscopy (XPS) and Infrared Reflection Absorption Spectroscopy (IRAS) using carbon monoxide (CO) as a probe molecule.
For Pt, both STM and IRAS results indicate that the (3x3)-MoO monolayer is the most promising candidate for stabilizing Pt single atoms, while small clusters and aggregates form on all other studied MoO_3 thin film phases already at room temperature. On the (3x3)-Mo_5O_8 monolayer films, the Pt atoms remain stable up to 500 K. Chemical characterization using XPS and IRAS shows that the Pt atoms remain electrically neutral rather than being oxidized, and that they bind carbon monoxide only weakly. These results will be compared with the stabilization of Ni atoms on the various MoO_3 films, for which a stronger interaction is expected.

ID	Title	Presenter	Type
639 **P100**	**Tuning Electronic Properties in 2D Covalent Organic Frameworks via On-Surface Chemistry**	Mira Sophie Arndt	Poster

Mira Sophie Arndt (1) Christoph Wachter (2) Roman Pallach (3) Yan Yan Grisan Qiu (4) Simone Mearini (4) Vitaliy Feyer (4) Sebastian Henke (3) Oliver Hofmann (2) Mirko Cinchetti (1) Giovanni Zamborlini (5)

(1) Department of Physics, TU Dortmund University
(2) Institute of Solid State Physics, Graz University of Technology
(3) Department of Chemistry, TU Dortmund University
(4) Peter Grünberg Institute (PGI-6), Jülich Research Centre
(5) Institute of Physics, University of Graz

Two-dimensional covalent organic frameworks (2D COFs) arranging in a Kagome lattice exhibit intriguing electronic properties, like flat bands and Dirac cones. We investigate the carbonyl-bridged aza-triangulene (P2TANGO), which assembles into a Kagome lattice on Au(111). Inspired by reports that deoxygenation of the precursor induces an open shell triplet ground state, we explore hydrogen-assisted deoxygenation to tune the COF's electronic properties. Our angle-resolved photoemission measurements reveal changes in the electronic structure upon oxygen removal, including energy shifts of the dispersive valence band features. DFT confirms that the shift grows with the deoxygenation, and that, in case of a complete deoxygenation, the degeneracy between the flat bands and the Dirac-dispersing bands is lifted.

ID	Title	Presenter	Type
334 **P101**	**Porphyrin Derivatives on Graphene Studied by STM**	Asma Khizar	Poster

Leonhard Grill (1) Asma Khizar (1) Christophe Nacci (1)

(1) Institute of Chemistry, University of Graz

Molecules as well as their assemblies and reactions have been widely investigated on single-crystal metal samples, which represent a defined flat support for efficient diffusion and high-resolution imaging by scanning probe microscopy (STM). However, the interaction between the metal and the molecule can alter the intrinsic properties of the molecules, making a decoupling layer essential to understand the pristine molecular properties. Graphene, with its two-dimensional structure and weak interaction with adsorbates, serves as an excellent decoupling layer for molecules. The reduced molecule-metal interaction allows the molecules to retain their intrinsic electronic features while still sensing the underlying metal, which influences adsorption energy and selective interactions. In this study, we used two surfaces as substrate for graphene growth: Cu(111) and Pt(111). The latter results in a Moiré pattern, enabling tuning of electronic decoupling and adsorption-site selectivity. Our focus is on chemical reactions of porphyrin derivatives on the graphene layer, thus at a distance from the metal catalysts.

560 P102	**$ZnFe_2O_4$-Based Electrochemical Sensors for Environmental Monitoring**	Hryhory Rymski	Poster

Hryhory Rymski (1) Mikhail Bunevich (2) Ilya Lagutskiy (3)

(1) Scientific and Practical Center for Materials Science of the National Academy of Sciences of Belarus
(2) Belarusian State University of Informatics and Radioelectronics
(3) ATOMTEX SPE

The development of highly sensitive and selective methods for the simultaneous determination of toxic heavy metal ions (HMIs), including Hg(II), Pb(II), and Cu(II), in environmental samples is one of the key challenges in modern electroanalysis, requiring novel electrode materials with enhanced adsorption and detection capabilities to address the issues of mutual interference and low sensitivity at trace concentration levels [1]. In this work, we propose the use of zinc ferrite nanoparticles (ZnFe2O4, ZFO), synthesized by the sol-gel method with subsequent calcination, as an effective electrode modifier to address this challenge.
The obtained ZFO nanoparticles possess a spinel structure, a small average size of approximately 11.2 nm, and a high specific surface area of 54.1 m2/g, as confirmed by X-ray diffraction (XRD) and transmission electron microscopy (TEM). The high specific surface area and well-developed mesoporous structure provide a large number of active sites for the adsorption of metal ions, which is a critical factor for the preconcentration step in stripping voltammetry.
Electrochemical studies using cyclic voltammetry (CV) and differential pulse anodic stripping voltammetry (DPASV) demonstrated that ZFO-modified electrodes exhibit significantly higher analytical signals compared to bare glassy carbon electrodes (GCE) or precursor-based electrodes.
Under optimized conditions (0.1 M HAc-NaAc buffer, pH=5.0, deposition potential -1.2 V, deposition time 120 s), the ZFO/GCE electrode showed excellent analytical performance for both individual and simultaneous determination of HMIs. The limits of detection (LOD, S/N=3) for simultaneous analysis reached 0.92 nM for Hg(II), 5.11 nM for Pb(II), and 7.84 nM for Cu(II). The electrode also demonstrated high reproducibility (relative standard deviation (RSD) < 1%), repeatability (RSD = 0.785% for 15 measurements of Hg(II)), stability over 7 days (RSD = 3.24%), and good selectivity in the presence of common interfering ions such as Al(III), Na(I), Ni(II), Co(II), and others. Successful testing on real water samples from a reservoir spiked with Hg(II) showed high recovery rates (97.7–102.4%), confirming the material's suitability for environmental monitoring applications.
Thus, ZnFe2O4 nanoparticles synthesized by the sol-gel method represent a promising material for the fabrication of electrochemical sensors intended for the sensitive and selective simultaneous determination of toxic heavy metal ions in natural and wastewater.

42 P103	**The Transient Phase of 1,1' Binaphthyl**	Sanjay John	Poster

Sanjay John (1) Anmol Andotra (1) Yves Geerts (2) Florian P. Lindner (1) Roland Resel (1) Ivo B. Rietveld (3) Rosanna Rizzi (4) Nina Strasser (1)

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(3) University of Rouen Normandy, Rouen, France
(4) Institute of Crystallography, Consiglio Nazionale delle Ricerch, Bari, Italy

The molecule 1,1'-binaphthyl is an axially chiral molecule that exists as two stable enantiomers which can change their conformation from one enantiomer to the other by overcoming a potential energy barrier of about 1 eV. Two types of crystallographic phases are known, one is racemic and the other is of chiral nature. We present an unknown type of phase which is obtained by rapid cooling from the melt with cooling rates larger than 10 °C/min. This new phase is formed also in thin films prepared by solution processing. The crystallisation process is studied by infrared thermography during melt crystallization, combined with differential scanning calorimetry and temperature-dependent in-situ X-ray powder diffraction. The new chiral phase crystallizes in the same space group $P4_12_12$ as the stable chiral phase, with slightly enlarged unit cell volume but with different molecular conformation. The new phase is unstable at room temperature and transfers into the stable chiral phase within few hours. This work demonstrates how crystallization kinetics influence the crystallization of conglomerates from a racemic melt or solution via a transient polymorphic state.

255 P104	**Self-Organized Surface Nanopatterning Induced by Ion Irradiation**	Denise Erb	Poster

Denise Erb (1) Stefan Facsko (1)

(1) Helmholtz-Zentrum Dresden-Rossendorf

The irradiation of a solid surface with a broad beam of low energy ions generates mobile vacancies and ad-atoms by erosive and ballistic effects. Surface erosion, ballistic and diffusive transport of the mobile ad-atoms and vacancies occur simultaneously and are each influenced by various system parameters. Due to this mass transport, the mobile species can self-assemble during continued ion irradiation into nanostructure patterns, following crystal structure, surface topography, and ion beam direction. Control of system parameters like the solid composition, crystal structure, surface temperature, ion mass and kinetic energy, or ion incidence angle allows for control of the resulting topographical pattern morphologies.
A wide variety of materials is sensitive to ion irradiation and a multitude of pattern morphologies with feature sizes in the range from some tens to a few hundreds of nanometers can be obtained. Investigations by AFM (ex-situ) and x-ray scattering (in-situ) show how they depend on the above system parameters and reveal the patterning dynamics. The patterning process is easy to implement and up-scaling the patterned surface area is straightforward. Applications can be found in nanopatterning by templating of various functional materials such as plasmonic structures, thermoelectrics, DNA origami, magnetic thin films, or catalysts.
We will present an introduction to ion-beam-induced surface nanopatterning, an overview of observed pattern morphologies and options for modification, as well as previously realized applications. We offer discussion on potential collaborations and exploration of further potential applications.

366 P105	**Fluorination Effects in Heptacene: From Gas Phase to Metal Interfaces**	Narjes Taghizadeh Rahaghi	Poster

Narjes Taghizadeh Rahaghi (1) Peter Puschnig (1) Andreas Windischbacher (1)

(1) Institute of Physics, University of Graz

Long acenes beyond pentacene are of considerable interest for organic electronics because their extended π-conjugation is associated with reduced energy gaps and enhanced charge carrier mobilities. At the same time, their pronounced reactivity and increasing open-shell character make their preparation and

characterization increasingly challenging [1,2]. In this contribution, heptacene is used as a long-acene system to investigate how fluorination can be employed as a chemically controlled route to tune molecular electronic structure and interface properties.
In the gas phase, fluorination induces a stabilization of the molecular orbital manifold due to the strong electron-withdrawing character of fluorine substituents, leading to an increase in electron affinity and a shift of the electronic spectrum toward lower energies [3]. This effect is directly reflected in core-level spectroscopy, where calculated C 1s binding energies shift toward higher values and exhibit a clear separation between chemically distinct C–F and C–C environments [3]. These gas-phase trends establish a well-defined reference for interpreting fluorination-induced modifications at interfaces.
We then consider adsorption on Ag(110) and Cu(110), two substrates with markedly different interaction strengths [4]. On Ag(110), where molecule–substrate coupling is comparatively weak, fluorination changes the balance between push-back and molecular dipole effects and reverses the sign of the work-function shift. On Cu(110), by contrast, stronger hybridization and charge redistribution dominate the interface electronic structure. The resulting changes are analyzed through the projected density of states (MOPDOS), which reveals how fluorination modifies frontier-orbital alignment and hybridization with the substrate.
These effects are further reflected in the simulated X-ray photoelectron spectra (XPS), which connect chemical substitution, charge transfer, and screening to observable C1s line-shape changes. Finally, we discuss C K-edge X-ray absorption spectroscopy (XAS/NEXAFS) as a natural extension of this framework. In combination with XPS, C K-edge XAS provides direct information on the unoccupied π* states and their evolution under fluorination and substrate interaction. Altogether, this study shows that fluorination is a powerful handle for tailoring vacuum-level alignment, hybridization, and spectroscopic fingerprints in acene-based interfaces.

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[2] Han J, Liu X, Li Y, Lou Z, Yi M, Kong H, Luo J. New synthetic approaches for hexacene and its application in thin-film transistors. Organic Chemistry Frontiers. 2019;6(16):2839-43.
[3] Bischof D, Radiev Y, Tripp MW, et. al. Chemical Doping by Fluorination and Its Impact on All Energy Levels of π-Conjugated Systems. The Journal of Physical Chemistry Letters. 2023 Mar 6;14(10):2551-7.
[4] Sättele MS, Windischbacher A,et al. Hexacene on Cu (110) and Ag (110): influence of the substrate on molecular orientation and interfacial charge transfer. The Journal of Physical Chemistry C. 2022 Mar 7;126(10):5036-45.

439 **P106**	**Electric Field Effects on the Adsorption of Redox Couples at Membrane Interfaces**	Agnes Maria Weiß	Poster

Agnes Maria Weiß (1) Stefan Spirk (1)

(1) Institute of Bioproducts and Paper Technology, Graz University of Technology, A-8010 Graz, Austria

Membranes play a vital role in systems exposed to electric fields, particularly in battery technologies, where they act as separators, preventing direct contact between electrodes while allowing controlled ion transport. In these environments, redox-active species, especially quinone-based redox couples, are known to interact with membrane surfaces, thereby influencing overall device performance. Such interactions can result in cross-diffusion of redox species, membrane fouling, and reduced ion-transport efficiency, including losses in proton conductivity. Despite their significance, the detailed interfacial behavior of redox-active species in the presence of electric fields remains an area that is still not fully understood, necessitating further investigation to improve membrane-based energy systems.
To address this gap, this study employs surface plasmon resonance (SPR) spectroscopy, a sensitive technique, to investigate these complex interactions. SPR enables real-time monitoring of adsorption processes on a variety of membrane materials and provides detailed insights into adsorption kinetics and changes in surface coverage over time. Moreover, SPR measurements clarify how the redox state of active species influences their interfacial behavior under different conditions. The experimental setup consists of an electrochemical flow cell equipped with a gold working electrode, a solid-state Ag/AgCl reference electrode, and a platinum counter electrode, enabling precise control of applied potentials. Through this setup, the study systematically compares the adsorption characteristics of redox-active species at the membrane interface both in the presence and absence of an external electric field, offering new perspectives on how electric fields modulate these phenomena.
Preliminary cyclic voltammetry analysis of the electrolyte has indicated species crossover, underscoring the necessity of understanding membrane–electrolyte interactions in these systems. The findings from this investigation are anticipated to provide valuable insights into the mechanisms by which redox-active species and electric fields collectively influence membrane interfaces. Ultimately, these insights will contribute to a deeper explanation of performance degradation in electrochemical systems, such as batteries and fuel cells, where membranes are critical components. By elucidating these interfacial phenomena, the study aims to inform the design of more robust and efficient membrane materials for future energy storage and conversion technologies.

541 **P107**	**Orthogonally Oriented Molecular Motors Assembled on the Surface: from Liquid-Solid to Ultrahigh Vacuum**	Robby Reynaerts	Poster

Robby Reynaerts (1) Steven De Feyter (2) Ben L. Feringa (3) Leonhard Grill (1) Cosima Stähler (3)

(1) Institute of Chemistry, University of Graz
(2) KU Leuven
(3) University of Groningen

Molecular motors continue to attract wide interest, due to their capability to convert energy into uni-directional rotary motion at the nanoscale. In solution, the rotational movement of the motors is overwhelmed by Brownian motion. However, one of the main challenges is to achieve organization of and cooperativity within multiple motor molecules to amplify the nanoscale motion and to use the motor's potential to do mechanical work on the macroscale to full capacity. In order to achieve this goal, the motors can, for example, be immobilized on a solid surface. Assembling such molecular motors and switches on a solid surface could impart a high degree of coherence in their orientation and packing. This leads to well-defined self-assembled molecular networks where the induced motion of the incorporated motors can be studied using state-of-the-art nanoscale imaging techniques such as scanning tunnelling microscopy (STM). Through molecular design such controlled assembly of molecular motors was achieved at the liquid-solid (LS) interface under ambient conditions. However, the inherent dynamics present at the LS interface were inseparable from the response of the molecular motors to external stimuli. Bringing the system over to low temperature and ultra-high vacuum (LT-UHV) conditions would rid any inherent dynamics from those ambient conditions. In this contribution I will discuss the controlled self-assembly of molecular motors on a solid surface achieved through molecular design under ambient and LT-UHV conditions and the experimental transition between these conditions.

1. Michl J. et al. Chem. Rev. 2005, 105, 1281−1376
2. Elemans J. et al. Soft Matter, 2012, 8, 9053
3. Feringa B.L. et al. Chem. Eur. J. 2024, e202303994

599 P108	**Deposition and Structural Characterization of Sol Gel Derived CeO_2:Ni Films**	Yasemin Caglar	Poster

Yasemin Caglar (1) Arsen Demiroglu (1)

(1) Eskisehir Technical University

Cerium dioxide (CeO_2) is one of the most studied materials due to its non-toxicity and environmental friendliness. The characteristic of its electronic structure, high UV absorption capacity, high refractive index and It is one of the most critical rare earth materials due to its high transparency in the visible region. These films are known to be used in electrochromic devices (ECDs) as passive counter electrodes and in lithium-ion batteries due to their excel-lent charge density and reversibility proper-ties. Several techniques were investigated to elaborate the CeO_2 thin films, such as magnetron sputtering, Microwave-assisted hydro-thermal, spin coating, electrochemical deposition, sol-gel, pulsed laser deposition, and spray pyrolysis technique. Among these methods, the sol–gel method is an attractive one due to its simplicity, safety, non-vacuum system of deposition, and inexpensive. Other advantages of this method are that it can be adapted easily for production of large-area films, and to get varying band gap materials during the deposition process.
In this study, Ni doped CeO_2 films were pre-pared by sol–gel process using a spin coating technique onto glass substrates. The crystal-line structure of the films were investigated by Xray diffractometer (BRUKER D2 Phaser). All the films of XRD patterns presenting the formation of the cubic CeO2 crystal structure (JCPDS reference 34-0394) having the polycrystalline nature. Diffraction peaks belong to (111), (200), (220), (311), (222), (400), (331) and (420) planes. The lattice constants, crystalline size and preferred orientation of the films were calculated from X-ray data.
Surface chemical composition and oxidation states were analyzed using X-ray photoelectron spectroscopy (XPS), confirming the successful incorporation of Ni into the CeO_2 lattice and providing insights into Ce^{3+}/Ce^{4+} ratios and oxygen vacancy formation. significantly influences the structural and defect characteristics of CeO_2 thin films.
Photoluminescence (PL) measurements of Ni-doped CeO_2 thin films were performed to understand the defect structure of these mate-rials.

600 P109	**Nickel Doped Cerium Oxide Films: Morphology and Optical Study**	Mujdat Caglar	Poster

Mujdat Caglar (1) Arsen Demiroglu (1)

(1) Eskisehir Technical University

Nickel (Ni) doped CeO_2 (Cerium Oxide) thin films and nanoparticles, fabricated via sol-gel, display enhanced functional properties such as increased oxygen storage capacity, higher optical transmittance, and improved conductivity, making them excellent for catalysts and sensors.
In this study, Ni doped CeO_2 films (3%, 5%,10%) using solutions were prepared by sol–gel process us-ing a spin coating technique onto glass substrates. Surface morphology and optical properties of the films were investigated by field emission scanning electron microscopy (ZEISS ULTRA PLUS) and UV Spectrophotometer including an integrating sphere attachment with using barium sulfonate as reference. (Shimadzu 2450), respectively.The influence of Ni doping on grain size, surface uniformity, and film density was systematically analyzed. Atomic force microscopy (AFM) was employed to obtain high-resolution topographical images and to quantify surface roughness parameters. AFM results confirmed the nanostructured nature of the films and showed that surface roughness varies with doping concentration, indicating changes in growth dynamics and film formation mechanisms.
In addition to morphological characterization, optical properties were investigated using UV–Vis spectroscopy. The optical transmittance and absorbance spectra were analyzed to determine key parameters such as optical band gap and optical constant (refractive index, extinction coefficient, dielectric constants). The results demonstrated that Ni doping leads to noticeable changes in optical behavior, including band gap modulation, which is attributed to defect states and structural modifications in the CeO_2 lattice.
Overall, the combined SEM, AFM, and optical analyses provide a comprehensive understanding of the relationship between surface morphology and optical performance, highlighting the potential of these thin films for applications in optoelectronic and photonic devices.

601 P110	**Investigation of Optical and Surface Properties of Ce-Doped NiO Thin Films Fabricated by Spin Coating Method**	Tülay Hurma	Poster

Tülay Hurma (1) Sabiha Aksay (1) Arsen Demiroglu (1)

(1) Eskisehir Technical University

Nickel oxide (NiO) thin films have attracted considerable attention due to their wide range of applications in advanced technologies, including transparent conducting oxides, gas sensors, photocatalytic systems, and optoelectronic devices. The ability to tailor their properties through doping provides a significant advantage for performance optimization. In particular, cerium (Ce) doping is of great interest as it enables tuning of the optical band gap and surface characteristics of NiO thin films.
In this study, undoped and 1%, 3%, and 5%Ce doped NiO thin films were deposited by sol gel spin coating method. Effects of Ce doping on the morphological and optical properties of the NiO films have been investigated. The surface morphology of the films were examined in detail using scanning electron microscopy (SEM) and atomic force microscopy (AFM). The analyses demonstrated that Ce doping significantly influences grain size, surface roughness, and morphological features. In particular, noticeable changes in surface structure were observed with increasing dopant concentration.
The optical properties were analyzed using UV-Vis spectroscopy, and the optical band gap values were determined from absorption spectra. The results revealed that the optical band gap of NiO thin films increased from 3.51 eV to 3.85 eV with increasing Ce doping concentration. The optical band constant values (refractive index, extinction coefficient, dielectric constants gap Urbach energy values) were determined.

611 P111	**Coordination, Geometry and Electronic Properties of a Bimetallic Porphyrin-Based Two-Dimensional Metal-Organic Framework on Au(100)**	Olga Resel	Poster

Olga Resel (1) Valentin Mischke (2) Mira Arndt (2) Claudia Obersnù (1) Michele Capra (2) Dominik Hruza (3) Iolanda Di Bernardo (4) Pierluigi Gargiani (5) Vitaly Feyer (6) Martin Sterrer (1) Mirko Cinchetti (2) Erik Vesselli (7) Giovanni Zamborlini (1)

(1) Institute of Physics, University of Graz
(2) Department of Physics, TU Dortmund University
(3) CEITEC - Central European Institute of Technology, Brno University of Technology
(4) Department of Condensed Matter Physics, Autonomous University of Madrid

(5) ALBA Synchotron Light Source
(6) Peter Grünberg Institute, Jülich Research Centre
(7) Department of Physics, University of Trieste

Metal-organic frameworks (MOFs) – porous periodic structures, consisting of metal nodes connected via organic linkers – offer a platform for designing materials with tailored electronic properties, owing to their modular chemistry. They host transition metal ions serving as active site for molecular binding, catalysis and magnetic applications. By employing a bottom-up approach on a suitable surface template, MOFs can be synthesized even at the 2D level. Here, I will present a thorough characterization of a porphyrin-based MOF, obtained by nickel deposition on self-assembled manganese tetrapyridylporphyrin (MnTPyP) on Au(100). A multi-technique approach combining low-energy electron diffraction, X-ray photoelectron and absorption spectroscopy, was employed to address the on-surface arrangement of the 2D-MOF, as well as the oxidation states of the metal nodes. Finally, angle-resolved photoemission spectroscopy (ARPES) allowed performing orbital tomography measurements and thus, accessing the geometrical and electronic properties of this 2D-MOF. In particular, we identify a $\left(5\sqrt{2} \times 5\sqrt{2}\right)$R45° 2D-MOF superstructure on Au(100). The symmetry match between MnTPyP and the substrate suppresses the formation of additional rotational domains, which is a significant advantage for ARPES analysis. The change of the resulting momentum maps indicates the formation of hybrid orbitals – a hallmark for MOF formation. For the metal-centers in the 2D-MOF, spectroscopic measurements point towards the +2 oxidation state in case of manganese, while nickel appears to be Ni(I). Overall, our results reveal the successful coordination of the molecules with nickel, yielding a well-ordered 2D-MOF with defined coordination geometry and electronic structure modifications at the metal centers.

686 **P112**	**Growth Study of Magnesium Oxide Islands and Thin Films on Ag(001)**	Maximilian Laßhofer	Poster

Maximilian Laßhofer (1) Jacek Goniakowski (2) Adriana Laufenböck (1) Claudine Noguera (2) Martin Sterrer (1)

(1) Institute of Physics, University of Graz
(2) Institut des Nanoscience de Paris, CNRS-Sorbonne Université

Magnesium oxide (MgO) thin films are widely used in surface science as insulating decoupling layers, substrates for metal particles, and model systems for studying charge transfer phenomena. While their functional properties have been extensively studied and several works on the growth of islands and films have been published, there still seems to be some uncertainty about the influence of different preparation parameters on the films' morphological and electronic properties.
In this work, we systematically investigate the early stages of MgO growth on Ag(001) using Scanning Tunneling Microscopy (STM) and X-ray Photoemission Spectroscopy (XPS). The influence of varying substrate temperature during growth under constant oxygen pressure is investigated, and vice versa. In submonolayer preparations, the optimal parameters yielding the stoichiometric growth of rectangular bilayer islands with edges running along the ⟨100⟩ directions have been identified. Under these conditions, the MgO islands are always embedded one layer deep in the Ag substrate. If the growth proceeds in magnesium excess – which is achieved by either lower O pressure or elevated temperatures – island growth favours ⟨110⟩ edges with additional Mg appearing at the MgO/Ag interface. This regime is additionally examined through Density Functional Theory (DFT), which provides further insights into edge stabilization mechanisms for stoichiometric and Mg-rich systems.
XPS in combination with observation of the secondary electron cutoff of XPS spectra have been applied to investigate the evolution of film thickness and workfunction from the early stages of island growth to the formation of thick, closed films. These investigations reveal the appearance of two growth regimes: (i) heteroepitaxial growth of islands until coalescence to a closed film occurs at a thickness of 3 ML, and (ii) homoepitaxial growth of MgO for thicknesses > 3 ML.

PIN - Physics - Industry

PIN – Session 1 (Thu 24, 10:30-12:30, Chairs: Peter Korczak / Christian Teissl)			
ID	Title	Speaker	Type
504	**Bridging Academic and Applied Physics: A Career in an RTO**	Borislav Hinkov	Invited talk (10:30-10:50)

Borislav Hinkov (1)

(1) Silicon Austria Labs

Studying physics opens many more career opportunities than academic research alone. Beyond universities, physicists play a key role in applied research institutions and research and technology organizations (RTOs), where fundamental scientific results and concepts are translated into industrial innovation and real-world applications.
In this talk, I will share my personal career path from physics studies and a PhD in experimental semiconductor physics, through academic research and university teaching, to my current role as senior researcher in integrated photonics at Silicon Austria Labs, while maintaining relevant ties to and collaborations with academia. Using selected examples from photonics and semiconductor device research, I will illustrate how skills developed in physics—analytical thinking, problem solving, experimental methodology, and interdisciplinary collaboration—translate naturally into industrially relevant applied research.
Particular attention will also be given to the experience of working across Germany, Switzerland, and Austria, and to the value of collaborating with colleagues from diverse cultural and professional backgrounds. These experiences illustrate the international and interdisciplinary nature of modern research careers.
The talk aims to demonstrate that a physics education opens diverse and rewarding career paths beyond the classical academic track, where RTOs offer an attractive environment for physicists who wish to combine scientific excellence with technological impact and application-driven innovation.

127	**Large Area Micro and Nanopatterning in Applied and Industrial Research**	Ursula Palfinger	Invited talk (10:50-11:10)

Ursula Palfinger (1)

(1) JOANNEUM RESEARCH Forschungsgesellschaft mbH

This talk presents a personal career pathway in applied research and industrial collaboration in the field of micro- and nanostructuring technologies. Ursula Palfinger began studying experimental physics at the Karl Franzens University Graz in 1998, later specializing in nanotechnology. An early opportunity to work in an industry-funded diploma project – on the microstructuring of optical elements via imprint lithography - sparked her long-term interest in applied physics and technology transfer.
Continuing along this path, she joined a European research project on printed electronics and completed her PhD in collaboration with JOANNEUM RESEARCH (JR). Her research focused on organic thin-film transistors, enhancing their electrical performance using nanoscale patterning. During this time, she gained extensive experience in structuring polymeric materials through both thermal (hot embossing) and UV-based imprint techniques, the latter offering distinct advantages in terms of process conditions and material multifunctionality.
As micro- and nanoimprint technologies matured, new application areas emerged, including freeform optics, microfluidics, and bio-inspired (bionic) surfaces. In response to the growing demand for large-scale manufacturing, her work contributed to the transition from small-scale laboratory processes to roll-to-roll (R2R) UV imprinting with meters-per-minute throughput. In this context, JR (Institute MATERIALS in Weiz) established Europe's first research pilot line for continuous large-area thermal and UV imprinting in 2010, enabling scalable prototyping and production of functional micro- and nanostructures.
A key technological challenge in R2R processing is the fabrication of large flexible tools used as imprint stamps, which led to the implementation of step-and-repeat type upscaling approaches. Ursula Palfinger has been technically responsible for this development and currently leads national and international research projects in this field.
The presentation will provide insights into selected applications and industry projects, highlighting both the scientific and practical aspects of this work. It aims to illustrate career opportunities available to physicists beyond academia, particularly at the interface of research, technology development, and industrial innovation.

85	**From Quantum Transport to Industrial Ion-Trap Systems**	Clemens Rössler	Invited talk (11:10-11:30)

Clemens Rössler (1)

(1) Infineon Technologies Villach

I will outline my path from physics studies and a PhD in Munich to ETH Zurich (postdoc and Oberassistent in quantum transport) with more than 50 peer-reviewed publications, then describe my move to Infineon Technologies in Villach in 2016. I will discuss the transition from MEMS process integration to leading Infineon's trapped-ion program, heading quantum technology development from 2020 and now serving as Senior Director Ion Trap Systems
I will present concrete outcomes: a team that today exceeds 50 people, co-developing quantum processing units with the leading system integrators; more than 50 patent families filed in trapped-ion quantum computing; industrially microfabricated ion traps produced in Villach; and a dedicated on-site quantum test laboratory.

92	**Kurzreferat PIN-session**	Georg Jakopic	Invited talk (11:30-11:50)

Georg Jakopic (1)

(1) JOANNEUM RESEARCH Forschungsgesellschaft mbH

Studium der Physik an der Technischen Universität Graz
Diplomarbeit und Dissertation zum Thema elektromagnetischer Wellenausbreitung in dünnen Festkörperschichten bzw. -systemen und Bestimmung optischer Konstanten am Institut für Theoretische Physik
Wechsel zur JOANNEUM RESEARCH Forschungsgesellschaft mbH (JR) an das neugegründete Institut für Nanostrukturierte Materialien und Photonik (NMP)
Aufbau optischer Analytik mit Spektrophotometrie und spektroskopischer Ellipsometrie
Themengebiete am Institut:
Organische Elektronik - insbesondere Feldeffekttransistoren und deren innere Interfaces
Charakterisierung von organischen Halbleiterstrukturen - speziell MIS-(Metall-Isolator-Halbleiter)-Strukturen
Mikro- und Nanostrukturierung mittels Ultrakurzpulslasersystemen
Optische Simulationen (Ray Tracing in unterschiedlichen Ausprägungen)
Physikalische Sensorik (piezo-/pyroelektrisch)
Überführung des NMP mit zwei weiteren Instituten von JR in das Institut für Sensorik, Photonik und Fertigungstechnologien (MATERIALS)
Es kommen folgende Arbeitsgebiete hinzu:
Rolle-zu-Rolle-basierte (skalierbare) Mikrostrukturierungsverfahren
Optochemische Sensorik (fluoreszenz- bzw. phosphoreszenzbasiert) - Ausbau des Themas hin zur Lab-on-Chip-basierten Diagnose
Aerosoljet-Druckprozesse
Inkjet-Druck in unterschiedlichen Ausprägungen (mit Verschmelzung mit dem NanoTecCenter Weiz (NTCW))
Dünnschichtabscheideprozesse (zunächst Pulsed-Laser-Deposition, Sputtern, dann zunehmend plasmagestützte Verfahren)
Metallurgie: Laserschweißtechnologien (inklusive Laserauftragsschweißen, Laserlegieren)

200	**Der Weg von der Grundlagenforschung zu Innovationen oder was eine Quantenphysikerin mit Erfindungen gemeinsam hat**	Marion Romirer	Invited talk (11:50-12:10)

Marion Romirer (1)

(1) Oesterreichisches Patentamt

Jeden Tag die neuesten technischen Innovationen serviert bekommen, noch bevor die restliche Welt davon erfährt? Und damit – zumindest teilweise – in die Fußstapfen eines der größten Physiker überhaupt treten? Klingt surreal? Nicht im Österreichischen Patentamt!
Denn wie schon Albert Einstein brüte ich als Patentprüferin täglich über diversen Erfindungen aus den verschiedensten technischen Gebieten. Zentral dabei ist die Beurteilung der Erfindungen hinsichtlich ihrer Neuheit und ihrer erfinderischen Tätigkeit. Dafür ist einerseits ein entsprechendes technisches Verständnis der Erfindung notwendig, andererseits aber auch eine gewisse Sprachgewandtheit sowie eine Brise Kreativität, um unter den Abermillionen an Patentschriften die relevantesten aufzuspüren.
Und nicht zuletzt verlangt die Arbeit als Patentprüferin, mich immer wieder in neue Themengebiete einzulesen – auch in solche, die fernab jener Themen liegen, mit denen ich mich während meines Physikstudiums an der Uni Wien beschäftigt habe. Neugierde und Offenheit Neuem gegenüber gehören also ebenfalls zu meiner täglichen Arbeit.
Offenheit und Neugierde waren es wohl letztlich auch, die mich vor fast genau fünf Jahren dazu bewogen, mich nach Abschluss meines Studiums für die Stelle als Patentprüferin zu bewerben, ohne eine genaue Vorstellung davon zu haben, was auf mich zukommen wird, da das Prüfen von Patenten – trotz prominenter Vorbilder – nicht unbedingt zu den gängigsten Karriereoptionen einer Quantenphysikerin zählt.
Wie sich mein Arbeitsalltag gestaltet, über welch absurd anmutende Erfindungen ich während meiner Recherchen stolpere und welche Aufstiegsmöglichkeiten es im Österreichischen Patentamt gibt, davon werde ich in diesem Vortrag erzählen.

400	**Psycho-Acoustics - From Cochlear Implant Development to Self-Administered Hearing Assessment**	Peter Schleich	Invited talk (12:10-12:30)

Peter Schleich (1) Josh Stohl (1)

(1) MED-EL Elektromedizinische Geräte GmbH

Psycho-acoustics can be found on the very basis of the development of cochlear implants. Several design features can be directly derived from psycho-acoustic experiments, like the number of electrode contacts, or the timing requirements of stimulation pulses. After bilateral cochlear implantation, psycho-acoustic methods are used to determine the effectiveness of the treatment.
My current working hypothesis: Inner ear hearing loss comes besides a reduction of amplification (through the loss of outer hair cell function) also with a broadening of auditory filters (a lack of population synchrony). This broadening can hardly be compensated for by acoustic amplification and signifies the sweet spot between hearing aid benefit and cochlear implant effectiveness.
Under development is an online tool running a streamlined 2-stage procedure, starting with a baseline test, followed by super-threshold psycho-acoustic tests.

YM – Young Minds

YM – Session 1 (Wed 23, 16:00-18:00, Chair: Anna Lena Busskamp) – Career Talks 1			
ID	Title	Speaker	Type
	Panel Discussion:		
	Career Paths Inside and Outside Academia		
	with		
	Plenary Speakers		
	Barbara Stadlober, Joanneum Research		
	and others		

YM – Session 2 (Thu 24, 16:00-18:00, Chair: Serafin Iwaniewicz) – Career Talks 2			
ID	Title	Speaker	Type
	Panel Discussion:		
	Work Life Balance in Physics		
	with		
	Ana Akrap, University of Zagreb		
	Anna Maria Coclite, University of Bari		
	Christian Hill, Brave Analytics		
	Rainer Minixhofer, AMS-Osram AG		

YM – Session 3 (Fri 25, 10:30-12:30, Chair: David Steiner) – YM Scholar Day			
ID	Title	Speaker	Type
811	**Award Talks of the Master thesis prizes 2026**	tba	
800	**The life cycle of a research idea**	Roberto Cerbini	

Roberto Cerbini (1)

(1) University of Vienna

Scientific discoveries usually reach us as finished products: a published paper, a conference talk, a breakthrough headline. Behind each one, though, lies a much longer and more uncertain journey. Before becoming a result, a research idea must compete for funding, attract people and resources, and survive experimental, theoretical, and computational dead ends. Most ideas never make it that far.In this talk, I will follow the life cycle of a research idea from its first spark to its dissemination and beyond. Along the way, we will see how research is funded and what obligations come with public and private money, how scientific teams are built, how peer review and publishing actually work, and why conferences and scientific communication matter as much as the results themselves. I will also be candid about the rejection and failure that are a normal part of the process. Seen together, these interconnected stages reveal modern science as a self-sustaining ecosystem, in which every result becomes the starting point for the next generation of ideas. My aim is to give early-career researchers a clearer (and more honest) picture of the scientific enterprise, and of everything that shapes research beyond the work itself.

437	**PLANCKS Austria: Competing, Connecting, and Changing Physics Education**	Johannes Krondorfer	

Johannes Krondorfer (1)

(1) TU Graz

Seven high-value physics problems, four hours, teams of up to four students: this was PLANCKS Austria 2026. Organized by PAULI in cooperation with ÖPG Young Minds as the national competition of the International Association of Physics Students, it brings together bachelor's and master's students to compete for a place at the international finals. In 2026, twenty teams tackled a diverse problem set spanning migratory-bird magnetoreception, graphene transport and Klein tunneling, neutrino oscillations, strong gravitational lensing, radiation of accelerated charges, and fundamental limits of silicon technology. Working collaboratively under time pressure, teams develop models, identify approximations, and structure solutions—mirroring core elements of real research and promoting learning through high-value, research-inspired problems. Formats such as "Students vs. Professors" and comparisons with ChatGPT and offline AI models add perspective, but the focus remains: physics is best learned by actively solving challenging problems together.

812	Space Team	Serafin Iwaniewicz	

YM – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
240 **P113**	**Investigating the Lithium Plateau with Gaia DR4 and Bayesian Regression**	Russell Huang	Poster

Russell Huang (1)

(1) Mountain View High School

The cosmological lithium problem is one of the biggest discrepancies between Big Bang nucleosynthesis predictions and stellar observations. In this paper, we measure the first Spite Plateau data with the latest GALAH DR4 survey. After we apply cuts to the data to isolate warm, metal-poor dwarf stars, we analyze lithium abundance compared to metallicity using the Bayesian regression code ROXY, which also accounts for uncertainties in Spite Plateau data. This allows us to calculate the slope, intercept, and scatter of Spite Plateau stars across varying metallicity cuts.
Across all metallicity cuts to [F e/H] < −2.0, the slopes remain at zero within uncertainties, confirming that the Spite Plateau has a flat relationship at low metallicity. These findings demonstrate that even with modern surveys and advanced Bayesian regression tools, there is no explanation for the Spite Plateau. Even with modern tools, the oldest stars appear to have near constant lithium with a strong discrepancy with the value expected from Big Bang Nucleosynthesis, which continues to be an open problem in cosmology and stellar astrophysics.

M01 - Electron Correlations and Phonons in Quantum Materials: A Theoretical and Computational Perspective

M01 – Session 1 (Wed 23, 10:30-12:30)			
ID	Title	Speaker	Type
55	**Shannon entropy and decoherence of polaron in metal halide perovskite pseudopotential quantum dot**	Alain Jerve Fotue	Invited talk (10:30-11:00)

Alain Jerve Fotue (1) Carlos Fotio (1) Francis Manfouo (1) Marius Silenou Mengoue (2) Roger M Keumo Tsiazec (3) S.L. Dongmo Tedoa (1)

(1) University of Dschang
(2) University of Douala
(3) University of Yaounde 1

In this work, we evaluated the eigen energies of the ground and first excited states of polaron, using Pekar type variational method, in pseudo-harmonic potential quantum dot. This was done with the aim of investigating the decoherence time and the Shannon entropy of the quantum dot in three different metal halide perovskites materials (MAPbCl3 , MAPbBr3, and MAPbI3). Numerical analysis results show that the decoherence time is an increasing function of the dot size, and dispersion coefficient of the phonon in each material. Additionally, the shannon entropy shows three different behaviors: messy behavior behavior for MAPbBr3, sinusoïdal behavior for MAPbCl3 materials and a near-sinusoïdal behavior for MAPbI3. These results suggest that, to construct a qubit from a quantum dot, it is essential to select a material with a suitable decoherence time.

736	**Comprehensive fluctuating field theory study of magnetic instabilities in the doped Hubbard model**	Erik Linnér	Invited talk (11:00-11:30)

Erik Linnér (1) Laura Torchia (1) Silke Biermann (2) Massimo Capone (3)

(1) Scuola Internazionale Superiore di Studi Avanzati
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Fluctuating field theory is a recently developed method for the description of competing collective fluctuations in correlated electron systems, able to account for spin, charge, and superconducting instabilities. On the basis of a variational principle, the method allows to explicitly account for the leading collective modes and their interplay, with access to electronic and spectroscopic properties. Extending its prior application to the Hubbard model at half-filling, we investigate its description of the doped Hubbard model, accounting for various spin instabilities. We show that unlike for Néel ordering, which dominates near half-filling, the phase structure of the fluctuating fields for collective instabilities with arbitrary ordering vector Q become important, expressing the modulation of the ordering relative the underlying lattice geometry. We observe the method, despite its weak-coupling rot, to give an efficient tool beyond mean-field theory to investigate a plethora of insulating and conducting magnetic phases with commensurate and incommensurate ordering vectors emerging within the phase diagram.

251	**Self-consistent two-particle calculations with quantics tensor trains -- solving the parquet equations**	Anna Kauch	Contributed talk (11:30-11:45)

Anna Kauch (1) Stefan Rohshap (1) Marc Ritter (2) Markus Wallerberger (1) Jan von Delft (3) Hiroshi Shinaoka (4)

(1) Institute of Solid State Physics, TU Wien
(2) CCQ Flatiron Institute
(3) Ludwig-Maximilian-University Munich
(4) Saitama University

Susceptibilities and optical conductivity are examples of two-particle response functions that are the key quantities for connecting theoretical predictions for correlated materials with experimental results. It can however become highly nontrivial to calculate them, especially in cases when nonlocal electronic correlations are important.
In my talk I will present a new computational approach to diagrammatic two-particle methods, namely the quantics tensor train representation [1], on the example of a set of self-consistent equations for two-particle vertex functions: the parquet equations. I will show that the steps needed to evaluate the equations (Bethe–Salpeter equations, parquet equation and Schwinger–Dyson equation) can be decomposed into basic operations on tensor trains. The repeated application of these operations does not lead to a loss of accuracy beyond a specified tolerance and the iterative scheme converges even for numerically demanding parameters. The applied methods allow for an exponential increase of the number of grid points included in the calculations, and a corresponding exponential reduction of the computational error, for a linear increase in computational cost [2].

[1] Phys. Rev. X 13, 021015 (2023)
[2] Phys. Rev. Research 7, 023087 (2025)

413	**Integrating non-Abelian structure in usual Euclidean lattices: Cayley Schreier lattices**	Lavi Kumar Upreti	Contributed talk (11:45-12:00)

Zoltán Guba (1) Tomas Bzdusek (1) Robert-Jan Slager (2) Lavi Kumar Upreti (1)

(1) University of Zurich
(2) University of Manchester

Most condensed matter physics happens on lattices with commuting translations—move right then up equals up then right. But hyperbolic lattices break this: translations become non-Abelian (NAB) or non-commutative, bringing remarkable physics—novel phases from single particle to many-body, superior quantum error correction. Problem: hyperbolic lattices need exponentially growing connections, impractical to scale.
We propose Cayley Schreier lattices (CSL): NAB translations in flat space without curvature. The trick is algebraic—replace each lattice site with n internal states corresponding to n group elements of a group. We will consider one such a group quaternion Q8

452	**DMFT calculations of electronic Raman scattering in layered ruthenates and rhodates**	Jernej Mravlje	Contributed talk (12:00-12:15)

Jernej Mravlje (1) Sophie Beck (2) German Blesio (3,4) Antoine Georges (5,6) Olivier Gingras (6,7)

(1) Jozef Stefan Institute
(2) TU Wien
(3) Instituto de Física Rosario (CONICET)
(4) Facultad de Ciencias Exactas, Ingeniería y Agrimensura, Universidad Nacional de Rosario, Rosario, Santa Fe, 2000, Argentina
(5) College de France
(6) CCQ Flatiron
(7) IPhT/CEA-Saclay

We investigate the electronic Raman scattering of Sr_2RuO_4 and Sr_2RhO_4 using a material-realistic dynamical mean-field theory approach. In the ruthenate compound we identify the low-energy Fermi liquid behavior and point out that the enhanced Raman response at higher energies is a fingerprint of Hund metals. These signatures originate in the two-stage coherence of Hund metals and associated quasiparticle `unrenormalization'. In rhodate compound we explain the origin of the unusually strong electronic Raman scattering peak at finite frequencies and offer a novel interpretation of the signal difference between different channels. We discuss the influence of spin-orbit and vertex corrections.

543	**$BaFe_2Se_3$: a quasi-unidimensional non-centrosymmetric superconductor**	Shiyu Deng	Contributed talk (12:15-12:30)

Shiyu Deng (1)

(1) Institut Laue-Langevin (ILL)

The spin-ladder compounds of the $BaFe_2X_3$ (X = chalcogen) family may be viewed as dimensional reductions—along stripe-like motifs—of the two-dimensional iron-based pnictide planes extensively studied since 2006. Remarkably, despite their reduced dimensionality, these materials retain the capacity for unconventional ground states, exemplified by the emergence of superconductivity in $BaFe_2Se_3$ under applied pressure beyond 10 GPa, following a structural phase transition at 4 GPa. Here, we report a comprehensive investigation combining high-resolution single-crystal X-ray diffraction, infrared spectroscopy, and ab initio calculations, which together elucidate the true crystallographic nature of this pressure-induced superconducting phase. While X-ray diffraction alone reveals a symmetry lowering from the widely accepted orthorhombic $Cmcm$ group to a monoclinic structure, it lacks sufficient sensitivity to resolve the precise space group. By integrating vibrational spectroscopy with density functional theory, we provide unambiguous evidence that the high-pressure phase is non-centrosymmetric, adopting the polar space group $P2_1$. These findings not only revise the structural assignment of $BaFe_2Se_3$ in its superconducting state but also establish its non-centrosymmetric character—an essential ingredient for potential unconventional pairing mechanisms—thereby opening new perspectives on the interplay between lattice symmetry, dimensionality, and superconductivity in iron-based materials.

[1] S. Deng, A. Roll, W.G. Zheng, G. Giri, T. Vasina, D. Bounoua, P. Fertey, M. Verseils, C. Bellin, A. Forget, D. Colson, P. Foury-Leylekian, M. B. Lepetit, and V. Baledent, Physical Review B, 113(12), L121105 (2026)

M01 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
494 **P041**	**Optical and acoustic polaron formation: Dynamic matrix approach (DMA)**	Martin Tchoffo	Poster

Martin Tchoffo (1) Jipi Nana (2) Lukon Corneliu (1)

(1) University of Dschang
(2) University of Bamena

This poster presents an all-coupling approach (dynamic matrix approach (DMA)) for the description of electron-phonon regimes. The model under investigation is based on an ionic crystal in which the electron-phonon coupling is modified by thermal excitations. The internal displacements of cations and anions as well as the resulting spontaneous polarization highlights the contributions of acoustic and optical phonon modes to Polaron formation. The electron-phonon Hamiltonian is therefore modified and a new quasi-particle is formed from the simultaneous interaction of the charge carrier with both acoustic and optical phonon modes. From this model, we gauge our method by comparison of the derived characteristics to well-known results (weak- and strong-coupling limit). It is observed that, the pyroelectric effect enhances the electron-phonon coupling and the combined contribution of both acoustic and optical modes leads to a composite polaron with a lager inertia.

M02 - Heavy Quasiparticles in Heavy Fermion Compounds

M02 – Session 1 (Tue 22, 16:00-18:00, Chair: Gertrud Zwicknagl)			
ID	Title	Speaker	Type
291	**Exploring Spin-Triplet Superconductivity in UTe_2 in Extreme Conditions**	Daniel Braithwaite	Invited talk (16:00-16:30)

Midori Amano Patino (1) Dai Aoki (2) Robert Borth (3) Daniel Braithwaite (4) Jean-Pascal Brison (4) Elena Hassinger (5) Georg Knebel (4) Gérard Lapertot (4) Michael Nicklas (3) Meike Pfeiffer (6) Gabriel Seyfarth (1) Timothée Vasina (4)

(1) Univ. Grenoble Alpes, CNRS, Institut Néel, F-38000 Grenoble, France
(2) Institute for Materials Research, Tohoku University, Oarai, Ibaraki, 311-1313, Japan
(3) Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany
(4) Univ. Grenoble Alpes, Grenoble INP, CEA, IRIG-Pheliqs, F-38000 Grenoble, France
(5) Institute for Quantum Materials and Technologies, Karlsruhe Institute of Technology, Kaiserstraße 12, 76131 Karlsruhe, Germany
(6) Institute for Solid State and Materials Physics, TU Dresden University of Technology, 01062 Dresden, Germany

Superconductivity in UTe_2 has many striking properties, like extremely high and anisotropic critical fields and the existence of multiple superconducting phases induced by either pressure or magnetic field. However perhaps the most unusual feature is the reinforcement of superconductivity in applied magnetic fields. The usual effect of magnetic field on superconductivity is through the effect of the field on the motion or the spin of the carriers. The effect of magnetic field on the pairing mechanism is absent or negligeable. This is not surprising in conventional superconductors where the pairing mechanism stems from the electron-phonon interaction, but it is also the case in most unconventional superconductors, even when the pairing mechanism has a magnetic origin. UTe_2 is one of the few exceptions where an applied magnetic field can enhance the strength of the pairing mechanism and actually reinforce superconductivity. In ambient pressure conditions, this effect is most spectacular when the field is applied along the b-axis of this orthorhombic system, where, above 15T, the superconducting critical temperature increases with increasing field. However under pressure a reinforcement of superconductivity with magnetic field is found for field applied along the c-axis. In both cases the probable origin is the proximity of a magnetic phase transition line that can be crossed by tuning the field. We will show recent calorimetry measurements in extreme conditions of pressure and/or magnetic field that reveal the interactions between the different phases and provide clues for the underlying pairing mechanisms for the unconventional superconducting phases of this fascinating material.

749	**Correlation induced quantum spin Hall insulating state in monolayer $TaIrTe_4$**	Honey Boban	Contributed talk (16:30-16:45)

Honey Boban (1) Tanguy Prongué (1) Felix Eder (1) Amarjyoti Choudhury (2) Fabian von Rohr (1) Marco Gibertini (2) Anna Tamai (1) Felix Baumberger (1,3)

(1) Department of Quantum Matter Physics, University of Geneva, Geneva, Switzerland
(2) Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Universita di Modena e Reggio Emilia, Modena, Italy
(3) Paul Scherrer Institute, Villigen, Switzerland

Monolayer $TaIrTe_4$ is theoretically predicted to be a quantum spin Hall insulator [1]. A recent transport study on monolayer TaIrTe4 has confirmed the insulating state at zero doping and reported edge conduction, consistent with a topological insulating state [2]. Intriguingly, a second insulating state with comparable edge conduction was found in gated samples where the chemical potential lies inside the non-interacting conduction band. This second insulating state was attributed to an electronic instability driven by saddle points van Hove singularities in the band structure.
I will present the first micro-focused angle-resolved photoemission spectroscopy (ARPES) results from monolayer $TaIrTe_4$. Our ARPES results confirm the insulating state of monolayer $TaIrTe_4$ and directly reveals the presence of van Hove singularities in the band structure.
In addition, I will also present preliminary results from bulk $TaIrTe_4$ and discuss their consistency with the putative type-II Weyl semimetal state predicted theoretically [3].

[1] P. J. Guo et al., Phys. Rev. B 102, 041109(R), 2020
[2] J. Tang et al., Nature 628, 515–521, 2024
[3] K. Koepernik et al., Phys. Rev. B 93, 201101(R), 2016

662	**Heterogeneous Ta-dichalcogenide bilayer: heavy fermions or doped Mott physics?**	Lorenzo Crippa	Contributed talk (16:45-17:00)

Lorenzo Crippa (1) Hyeonhu Bae (1) Igor I. Mazin (2) Giorgio Sangiovanni (1) Roser Valenti (1) Tim Wehling (1) Binghai Yan (1)

(1) University of Hamburg
(2) George Mason University

Controlling and understanding electron correlations in quantum matter is one of the most challenging tasks in materials engineering. In the past years a plethora of new puzzling correlated states have been found by carefully stacking and twisting two-dimensional van der Waals materials of different kind. Unique to these stacked structures is the emergence of correlated phases not foreseeable from the single layers alone. In Ta-dichalcogenide heterostructures made of a good metallic “1H”- and a Mott-insulating “1T”-layer, recent reports have evidenced a cross-breed itinerant and localized nature of the electronic excitations, similar to what is typically found in heavy fermion systems.
Here, we put forward a new interpretation based on first-principles calculations which indicates a sizeable charge transfer of electrons (0.4-0.6 e) from 1T to 1H layers at an elevated interlayer distance. We accurately quantify the strength of the interlayer hybridization which allows us to unambiguously determine that the system is much closer to a doped Mott insulator than to a heavy fermion scenario.

225	**Change in charge density wave order beyond the Lifshitz transition in 2H-$Ta_{1\pm\delta}S_2$**	Mihir Date	Contributed talk (17:00-17:15)

Mihir Date (1) Jan Berges (2) Enrico Da Como (3) Alex Louat (4) Marcin Mucha-Kruczyn'ski (3) Gabriele Domaine (1) Niels Schroeter (1) Malte Roesner (5) Matthew Watson (4)

(1) Max Planck Institute of Microstructure Physics
(2) Universitaet Bremen
(3) University of Bath
(4) Diamond Light Source Ltd.
(5) Radboud University

We investigate electronic instabilities in 2H-TaS and a self-intercalated variant, 2H-TaS. In conventional samples, which we determine to be slightly hole-doped, spectral gaps and backfolded features are found as fingerprints of the 3×3 charge density wave (CDW). Notably, the backfolded features emerge only at a temperatures below $T \approx 65$ K, substantially lower than the established CDW temperature of 78 K, suggesting an incommensurate-commensurate lock-in transition analogous to the phenomenology of the 2H-TaSe. In contrast, the self-intercalated 2H sample exhibits substantial electron doping and signatures of a novel $2\sqrt{3} \times 2\sqrt{3}R(30^\circ)$ CDW. Using ab initio calculations of the phonon spectrum, we demonstrate that the 3×3 instability ($\mathbf{q} = \frac{2}{3}\mathbf{\Gamma M}$) is highly sensitive to band filling. Furthermore, with increased interlayer spacing, a competing soft phonon mode emerges near $\mathbf{q} = \frac{1}{2}\mathbf{\Gamma K}$, corresponding to the superstructure observed in the 2H phase, although in our calculations this instability arises under hole doping rather than the electron doping inferred experimentally. These results establish band filling and interlayer spacing as key control parameters for CDW ordering vectors in 2H-TaS, and highlight a route to engineering electronic instabilities in a prototypical layered material.

652	**Influence of higher-order Van Hove singularities on superconductivity-induced Kondo destruction**	Grzegorz Michałek	Contributed talk (17:15-17:30)

Grzegorz Michałek (1) Krzysztof P. Wójcik (1)

(1) Institute of Molecular Physics, Polish Academy of Sciences

In quantum materials research, exploiting electronic interactions is key to tuning systems toward interesting phases. However, describing correlations in interacting lattice systems remains notoriously difficult, posing challenges for both precise theoretical descriptions and the interpretation of experimental data. In this work, we investigate the effect of higher-order Van Hove singularities (HOVHS) on a single magnetic impurity embedded in a superconducting host. This system serves as a promising platform, as it is accessible to both advanced theoretical methods and high-precision scanning tunneling microscopy (STM) experiments, allowing for reliable and verifiable predictions.
The physics of magnetic impurities in superconductors is governed by the competition between Kondo screening and superconducting pairing. This interplay typically drives a quantum phase transition between a screened singlet ground state and an unscreened phase, the latter being characterized by the formation of Yu-Shiba-Rusinov (YSR) in-gap states [1,2]. Using numerical renormalization group calculations, we demonstrate that the quantum critical point shifts toward larger values of the superconducting pairing strength with an increasing singularity exponent. Our findings indicate that the tuning of Van Hove singularities is a potential mechanism for controlling quantum phase transitions in doped superconductors.

[1] K. Satori, H. Shiba, O. Sakai, Y. Shimizu, J. Phys. Soc. Jpn. 61, 3239 (1992).
[2] C. P. Moca, I. Weymann, M. A. Werner, G. Zaránd, Phys. Rev. Lett. 127, 186804 (2021).
This work was supported by the National Science Centre, Poland, under project No. 2023/51/D/ST3/00532.

792	**Fermi surfaces and electronic structure of uranium-based superconductors**	Alix McCollam	Invited talk (17:30-18:00)

A. McCollam (1) R. Leenen (2) D. Aoki (3) G. Knebel (4) S.R. Julian (5) A. Pourret (4)

(1) School of Physics, Kane Building, University College Cork, College Road, Cork, Ireland
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(3) Institute for Materials Research, Tohoku University, Ibaraki 311-1313, Japan
(4) Univ. Grenoble Alpes, CEA, Grenoble INP, IRIG, PHELIQS, F-38000 Grenoble, France
(5) Department of Physics, University of Toronto, 60 St. George Street, Toronto, M5S 1A7, Ontario, Canada

Lifshitz transitions of the Fermi surface are significant in a wide variety of strongly correlated and topological materials, and understanding the origin and influence of Lifshitz transitions has led to deeper understanding of key aspects of magnetic, transport or quantum critical behaviour.
In the ferromagnetic superconductor UCoGe, a magnetic field applied along the c-axis induces a series of anomalies in both transport and thermopower that may be caused by Lifshitz transitions. A need to understand the close relationship between magnetism, superconductivity and the heavy electron Fermi surface in this material makes it important to explore if and why such a series of magnetic-field-induced Lifshitz transitions occur. Lifshitz transitions are also prominent at high magnetic fields in UPt and UTe.
I will discuss the results of magnetic susceptibility measurements of UCoGe, in magnetic fields up to 30 T, in which we observed a series of clearly-defined features in the susceptibility, and multiple sets of strongly field-dependent de Haas-van Alphen oscillations. From the experimental results complemented by DFT bandstructure calculations, we extracted detailed field-dependence of the quasiparticle properties, determined the likely shape of the Fermi surface and identified candidate Lifshitz transitions.
e results from UCoGe to other recent Fermi surface measurements of UPt and UTe, and discuss the evolution of the Fermi surface in connection to the development of magnetisation and superconductivity in these materials.

M02 – Session 2 (Wed 23, 16:00-18:00, Chair: Markus Aichhorn)			
ID	Title	Speaker	Type
77	**Anisotropic spin Hamiltonians and low-temperature magnetic phases in rare-earth triangular-lattice compounds**	Leonid Pourovskii	Invited talk (16:00-16:30)

Leonid Pourovskii (1)

(1) CPHT, CNRS, Ecole polytechnique, IP Paris, 91120 Palaiseau France

Rare-earth triangular-lattice compounds stand as prime candidates for harboring exotic quantum spin liquid (QSL) phases, but their effective low-energy Hamiltonians and magnetic ground states remain difficult to determine experimentally. We evaluate ab initio effective spin-1/2 Hamiltonians for a set of Ce and Yb triangular lattice compounds from their paramagnetic electronic structure using the force theorem in Hubbard-I method. This force-theorem approach is generalised to include, apart from 4 kinetic exchange, also indirect exchange induced through the 4-5 on-site Coulomb interaction. The resulting Hamiltonians are solved using either single-site quantum mean-field or exact diagonalization of finite-size clusters. For the triangular lattice Ce delafossites CsCeSe, KCeS, and RbCeO, we find that the indirect exchange dominates in the selenide, the kinetic exchange in the oxide, while both mechanisms contribute almost equally in the sulfide. Overall, we find conventional ordered magnetic ground states for all studied compounds, including some putative QSL candidates. Our findings highlight a possibly important role of deviations from the perfect triangular model—like atomic disorder—in real triangular-lattice materials.

[1] L. V. Pourovskii, R. Soares, A. Wietek, Phys. Rev. B 113, L060401 (2026).
[2] L. V. Pourovskii, arXiv:2511.14904.

734	**Quantum Fisher information in a strange metal**	Federico Mazza	Contributed talk (16:30-16:45)

Sounak Biswas (1) Federico Mazza (2) Fakher Assaad (1) Silke Paschen (3) Andrey Prokofiev (2) Qimiao Si (4) Paul Steffens (5) Xinlin Yan (2)

(1) Institut für Theoretische Physik und Astrophysik, Universität Würzburg, 97074 Würzburg, Germany
(2) TU Wien
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Strange metal behavior emerges across a wide range of material platforms and remains a central open problem in correlated quantum matter [1]. Beyond the hallmark linear-in-temperature electrical resistivity, it is characterized by entropy accumulation, a discontinuous change in Fermi volume, and energy-over-temperature scaling in dynamical susceptibilities [2]. Recent studies suggest that kagome metals, hosting flat electronic bands near the Fermi level, can exhibit magnetic-field-tunable strange metal behavior even in the absence of f electrons [3]. The heavy fermion compound Ce3Pd20Si6 provides an ideal platform to investigate quantum criticality beyond the Landau–Ginzburg–Wilson framework, including access to fractional critical exponents and emerging concepts such as multipartite entanglement [4,5]. Here, we present inelastic neutron scattering measurements at a strange-metal quantum critical point in Ce3Pd20Si6. Our analysis reveals dynamical scaling behavior, quantifies the entanglement depth via the quantum Fisher information density fQ, and establishes a direct comparison with quantum Monte Carlo simulations. These results highlight intriguing connections between heavy-fermion systems and flat-band materials [3,6].

[1] Checkelsky, J. G., et al. Flat bands, strange metals, and the Kondo effect, Nat. Rev. Mater. 9, 509–526 (2024).
[2] Paschen, S. & Si, Q. Quantum phases driven by strong correlations, Nat. Rev. Phys. 3, 9–26 (2021).
[3] Ye, L., et al. Hopping frustration-induced flat band and strange metallicity in a kagome metal. Nat. Phys. 20, 610–614 (2024).
[4] Martelli, V., et al. Sequential localization of a complex electron fluid, Proc. Natl. Acad. Sci. U.S.A. 116, 17701 (2019).
[5] Hauke, P., et al. Measuring multipartite entanglement through dynamic susceptibilities, Nat. Phys. 12, 778–782 (2016).
[6] Mazza, F., Biswas, S., et al. Quantum Fisher information in a strange metal, arXiv:2403.12779 to appear in Nat. Phys. (2026).

700	**Topological semimetal in a quantum critical heavy fermion system**	Diana M. Kirschbaum	Contributed talk (16:45-17:00)

Diana M. Kirschbaum (1) Lei Chen (2) Diego A. Zocco (1) Haoyu Hu (2) Federico Mazza (1) Matthias Karlich (1) Monika Lužnik (1) Duy Ha Nguyen (1) Julio Larrea Jiménez (1,3) André M. Strydom (4) Devashibhai Adroja (5) Xinlin Yan (1) Andrey Prokofiev (1) Qimiao Si (2) Silke Paschen (1)

(1) Institute of Solid State Physics, TU Wien
(2) Rice University
(3) University of São Paulo
(4) University of Johannesburg
(5) ISIS Neutron and Muon Source, Rutherford Appleton Laboratory

Strongly correlated electron systems are known to exhibit a range of exotic phenomena, including strange metal behavior and unconventional superconductivity [1]. More recently, they are also discussed in the context of nontrivial band topology [2]. As the standard formulation of the latter relies on well-defined quasiparticles, one may ask whether topological characteristics can persist in regimes where the conventional band-structure description breaks down. Heavy fermion systems provide a natural setting to address this question, as quantum criticality of beyond order parameter type [1] and Weyl-Kondo semimetal behavior [3-5] have both been observed. Here, we study the non-centrosymmetric heavy fermion compound CeRuSn, which is intrinsically quantum critical [6]. Our experiments reveal a topological semimetal phase emerging from the quantum critical regime, with a dome-like dependence on pressure and magnetic field. These results are understood by generalizing the concept of Weyl crossings to non-quasiparticle spectral functions overlapping at specific positions in momentum space [7]. This mechanism may also occur in other quantum critical systems of suitable symmetry, suggesting a new design principle for emergent topological phases.

[1] S. Paschen and Q. Si, Nat. Rev. Phys. 3, 9 (2021).
[2] J. G. Checkelsky et al., Nat. Rev. Mater. 9, 509 (2024)
[3] S. Dzsaber et al., Phys. Rev. Lett., 118, 246601 (2017)
[4] H.-H. Lai et al., Proc. Natl. Acad. Sci. U.S.A. 115, 93 (2018)
[5] S. Dzsaber et al., Proc. Natl. Acad. Sci. U.S.A. 118, e2013386118 (2021)

[6] W. T. Fuhrman et al., Sci. Adv. 7, eabf9134 (2021)
[7] D. M. Kirschbaum, L. Chen et al., Nat. Phys. 2, 218 (2026)
This work was supported by the Austrian Science Fund (FWF grants I4047, SFB F 86 “Q-M&S”, and I5868-N/FOR 5249 "QUAST"), the European Microkelvin Platform (H2020 project 824109), the European Research Council (ERC Advanced Grant 101055088-CorMeTop), and the US AFOSR (Grant FA8655-24-1-7018).

93	**Intertwining bulk and surface: The case of UTe_2**	Aline Ramires	Invited talk (17:00-17:30)

Aline Ramires (1) Andras Szabo (2)

(1) TU Wien
(2) MPI-FKF

UTe_2 has been the focus of numerous experimental and theoretical studies in recent years, as it is recognized as one of the few odd-parity bulk superconductors. Its surface has also been probed, revealing charge density wave (CDW), pair density wave, and time-reversal symmetry breaking (TRSB). Here, we propose that the interplay between bulk and surface order parameters in UTe_2 may be crucial in explaining its unusual surface properties. Through a phenomenological analysis, assuming a dominant CDW, we can account for three distinctive experimental signatures: (1) the apparent suppression of CDW order at the upper critical field of the bulk superconducting state; (2) the magnetic-field-induced imbalance of the Fourier peaks associated with the CDW; and (3) the onset of TRSB with bulk superconductivity and its field trainability. Furthermore, we propose specific experiments to validate our conjecture, which we believe could be promptly achieved.

782	**Thermodynamic Probes of Hidden Superconducting Phase Boundaries in UTe_2**	Michal Vališka	Invited talk (17:30-18:00)

M. Valiska (1) T. Haidamak (1) A Cabala (1) V. Sechovsky (1) P. Proschek (1) A. Hauspurg (2) S. Zherlitsyn (1)

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UTe_2 is one of the most prominent candidate materials for spin-triplet and potentially topological superconductivity. Its superconducting phase diagram is exceptionally rich, with multiple field- and pressure-induced phases whose topology remains intensely debated. A particularly important unresolved issue concerns the high-field superconducting regime for magnetic field applied along the hard b axis. Previous ac-susceptibility and transport studies suggested an internal superconducting phase boundary near 14–15 T [2,3], but clear bulk thermodynamic evidence for this boundary had been missing.
This work presents high-field ultrasound measurements on ultraclean UTe_2 single crystals with Tc above 2 K [1]. By measuring several elastic modes in static magnetic fields up to 18 T and temperatures down to 0.33 K, we identify a distinct anomaly in the longitudinal C_{33} mode near 14–15 T. A weaker response is observed in C_{44}, whereas no corresponding anomaly is resolved in C_{55}. This mode selectivity demonstrates that the high-field superconducting state couples anisotropically to lattice strain and provides symmetry-sensitive constraints on the superconducting order parameter.
The observed elastic anomaly supplies the missing bulk thermodynamic evidence for the internal superconducting phase line. This line terminates near 13.5 T and 1.25 K at a tetracritical point, completing the local four-boundary topology of the H–T phase diagram for H ∥ b [1]. The results support field-induced multicomponent superconductivity in UTe_2 and connect the ambient-pressure high-field phase diagram to the recently established pressure-induced tetracritical regime [4]. More broadly, they demonstrate the power of ultrasound to reveal hidden superconducting phase boundaries that may remain weak or unresolved in specific heat.

[1] M. Vališka et al., arXiv: 2604.25896 (2026).
[2] H. Sakai et al., Physical Review Letters 130, 196002 (2023).
[3] Y. Tokiwa et al., Physical Review B 108, 144502 (2023).
[4] S. Kamat et al., arXiv:2603.17905 (2026).

M02 – Session 3 (Thu 24, 16:00-18:00, Chair: Carolina A. Marques)

ID	Title	Speaker	Type
780	**STM Measurements of Topology and Gap Symmetry of the Heavy Fermion Superconductor UTe_2**	Vidya Madhavan	Invited talk (16:00-16:30)

Vidya Madhavan (1)

(1) Department of Physics and Materials Research Laboratory, University of Illinois Urbana-Champaign, Urbana, IL, USA

One of the central open questions in the heavy fermion triplet superconductor UTe_2 concerns the nature of the quasiparticles within the superconducting gap which make the gap unusually shallow. A compelling possibility is that the gap appears shallow because the nontrivial topology in UTe_2 gives rise to in-gap surface states. A persuasive proof of this would be the gapping of the in-gap surface states upon breaking the symmetry that protects the topological states.
In this talk I will discuss our recent vector magnetic-field scanning tunnelling microscopy studies of UTe_2. Atomic-scale spectroscopy reveals striking site-dependent superconductivity: Te sites host a large in-gap density of states that nearly fill the superconducting gap, whereas neighboring atomic sites remain gapped. We find that the application of a magnetic field suppresses the in-gap states on the Te sites, yielding a spatially homogeneous superconducting state with a markedly enhanced average gap depth relative to zero field. This site-selective gap deepening is in quantitative agreement with theoretical predictions for topological surface states in UTe_2 that possess dominant Te-orbital character within a point-nodal triplet superconducting state. Spectral-function calculations incorporating the Zeeman coupling reproduce the observed magnetic-field response. Our results provide direct spectroscopic evidence of the existence of topological surfaces in the superconducting phase of UTe_2 and establish this strongly correlated superconductor as a promising platform for exploring intrinsic topological superconductivity.

694	**Determining the superconducting order parameter of UPt_3 using scanning tunneling microscopy**	Peter Wahl	Contributed talk (16:30-16:45)

Rebecca Bisset (1) Luke Rhodes (1) Hugo Decitre (1) Matthew Neat (1) Ana Maldonado (1) Andrew Huxley (2) Carolina de Almeida Marques (1) Peter Wahl (1)

(1) University of St Andrews
(2) University of Edinburgh

Superconductivity emerges due to pairing of electrons in Cooper pairs, which are bosonic quasi-particles with integer spin and which condense into a macroscopically coherent ground state. So far, in all cases where the pairing symmetry of the Cooper pairs has been established, they form a spin singlet state, but they could in principle also exist as spin one quasi-particles and form a spin-triplet condensate.
The currently leading candidate materials are the uranium superconductors, however identifying their pairing symmetry has remained challenging. I will show a detailed study of the candidate triplet superconductor UPt_3 by scanning tunneling spectroscopy, and how from a combination of tunneling spectroscopy and theoretical modelling we can draw conclusions about the superconducting order parameter.

615	**Imaging tuning of electronic structure with chemical pressure in $Sr_{2-x}Ba_xRuO_4$**	Siri A. Berge	Contributed talk (16:45-17:00)

Siri A. Berge (1) Rebecca Bisset (1) Daniel Halliday (1) Carolina de Almeida Marques (1) Luke C. Rhodes (1) Alexander C. Komarek (2) Phil D. C. King (1) Peter Wahl (1)

(1) University of St Andrews
(2) Max Planck Institute for Chemical Physics of Solid

Tuning the electronic structure of layered perovskites is a powerful pathway to control their properties for future applications. The electronic structure of Sr_2RuO_4 can be controlled by small structural distortions, with in-plane rotations of the oxygen octahedra moving the van Hove singularity across the Fermi level. This Lifshitz transition is expected to result in significant consequences for the ground state and the properties of the superconductivity [1-2]. Here, we study the effect of chemical pressure by substitution with isovalent Ba atoms in $Sr_{2-x}Ba_xRuO_4$ for x = 0, 0.2, and 0.4 by Scanning Tunnelling Microscopy (STM). We report a systematic study of the structural and electronic changes with substitution level. Despite the substitution being isoelectronic and away from the electronically active RuO_2 plane, our results show substantial inhomogeneity of the electronic structure close to the Fermi energy. Our results highlight the connection between electronic and lattice degrees of freedom and demonstrate control of the electronic structure.

[1] Marques, C. A. et al. Advanced Materials 33, 2100593 (2021).
[2] Profe, J. B. et al. Phys. Rev. Research 6, 043057 (2024).

725	**Intertwined Electronic Phases in the Type-II Weyl Semimetal WTe_2**	Alexander LaFleur	Contributed talk (17:00-17:15)

Kevin Hauser (1) Alexander LaFleur (1) Rian Ligthart (1) Fabian Natterer (1) Gleb Neplyakh (1)

(1) Universität Zürich

The candidate type-II Weyl semimetal WTe_2 has been shown to host electron-hole band crossings, unusually large magnetoresistance, and nanoscale ferroelectric domains, but there is a lack of experimental evidence establishing the connection between these different phases. While most ferroelectric materials are insulators, WTe_2 is a semimetal, and because of this poses a unique opportunity to study the interplay of these phases by nanoscale imaging using scanning tunneling microscopy/spectroscopy (STM/S). Here, we characterize the different domain and impurity types which inhabit the nanoscale landscape of WTe_2 to elucidate the correlations between electron and hole pockets of the Fermi surface, magnetism, ferroelectric domains, and the Type-II Weyl points. Mapping of the real space scattering of the Fermi surface electron and hole pockets shows correlations between impurities, ferroelectric domains, DC offsets, strain, and magnetism.

675	**High-Resolution QPI Study of Electronic States in Bulk WTe_2**	Rian Ligthart	Contributed talk (17:15-17:30)

Rian Ligthart (1) Alexander LaFleur (1) Gleb Neplyakh (1) Kevin Hauser (1) Fabian Natterer (1)

(1) Universität Zürich

Transition Metal Dichalcogenides (TMDs), a key class of 2D quantum materials, are emerging as promising alternatives to enhance efficiency at the same length scale as silicon-based electronics. Among them, WTe_2 stands out for its unique bulk properties, including its topological semimetal behaviour, the type II Weyl fermions it hosts, and its exceptionally large magnetoresistance.
We investigate cleaved bulk WTe_2 using a scanning tunneling microscope (STM) at 330 mK, combining with scanning tunnelling spectroscopy to probe its electronic properties and their dependence on vector magnetic fields. By applying sparse sampling techniques, we resolve new QPI wavevectors in WTe_2, shedding a new light on the electronic band structure of this interesting material.

462	**Theory of superconducting pairing and topological surface states in UTe_2**	Brian Moller Andersen	Invited talk (17:30-18:00)

Brian Moller Andersen (1)

(1) Niels Bohr Institute, University of Copenhagen

The heavy-fermion compound UTe_2 is a candidate for hosting intrinsic spin-triplet superconductivity. At present, however, the type of triplet Cooper pairing realized in UTe_2 remains unknown, which calls for further experimental and theoretical investigations. In this talk, I present a microscopic minimal model for the superconducting phases of UTe_2 based on recent findings in the description of its low-energy normal state electronic properties. I apply the resulting

theoretical model to extract the nodal gap properties of the allowed superconducting ground states, and deter-mine their associated topological surface states on the experimentally relevant (0-11) cleave plane.

It is found that the Fermi surface of UTe_2 enforces additional point nodes in excess to the point nodes imposed by symmetry, which may reconcile several experiments seemingly in conflict with B2u or B3u pairing symmetries. Furthermore, we map out the in-gap Majorana surface-bound modes exist-ing on the (0-11) surface, and discuss their potential for additional insight into the pairing structure of UTe_2. Quasiparticle interference (QPI) obtained from scanning tunneling microscopy (STM) is a pow-erful method to help extract the pairing symmetry of unconventional superconductors. We apply the model for UTe_2 to compute its QPI signals and compare the resulting QPI with recent STM measurements. We conclude that the two candidate Cooper pair instabilities B2u and B3u exhibit distinct features in the QPI intensity to discriminate these using the experimental data. Characteristic features of the emergent topological surface states protected by mirror symmetries provide further unique signatures to help pinpointing the pairing symmetry channel of UTe2. I will discuss to what extent experimental STM results are in agreement with various proposed pairing states of UTe_2.

M02 – Poster session (PS1 Mon21-Tue22)			
ID	Title	Presenter	Type
790 **P001**	**Superconducting density of states and vortex lattice of $LaRu_2P_2$ and superconducting gap of $SrBi_2Se_4$**	Paula Obladen Agilera	Poster

Marta Fernandez-Lomana (1) Paula Obladen Agilera (1) Beilun Wu (1) Edwin Herrera (1) Hermann Suderow (1) Isabel Guillamon (1)

(1) Laboratorio de Bajas Temperaturas, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, Madrid, Spain

We provide the superconducting density of states of the pnictide superconductor $LaRu_2P_2$, measured using millikelvin scanning tunnelling microscopy. From the tunnelling conductance, we extract a density of states which shows the opening of a s-wave single superconducting gap. The temperature dependence of the gap also follows BCS theory. Under magnetic fields, vortices present Caroli de Gennes Matricon states, although these are strongly broadened by defect scattering. $SrBi_2Se_4$ can be viewed as a structurally and electronically derived system from Bi_2Se_3, where the fundamental Bi–Se building blocks found in the layered topological insulator Bi_2Se_3 are reconfigured into a quasi-one-dimensional framework, leading to anisotropic properties and potentially modified topological behaviour compared to the parent 3D compound. Contrary to Bi_2Se_3, $SrBi_2Se_4$ is superconducting and could host correlations, due to its low-dimensional structure, and potential topological properties. Here we present first measurements of the superconducting gap of $SrBi_2Se_4$ as a function of temperature.

[1] Marta Fernández-Lomana et al 2025 J. Phys.: Condens. Matter 37 025604

M03 - Correlated Materials Out of Equilibrium

M03 – Session 1 (Mon 21, 10:30-12:30, Chair: Martin Eckstein)			
ID	Title	Speaker	Type
62	**Electron Correlation Effects on the Electronic Structure and Spin Transport Properties of Spintronic Devices Beyond Linear Response**	Andrea Droghetti	Contributed talk (10:30-10.45)

Andrea Droghetti (1) Liviu Chioncel (2) Declan Nell (3) Milos Radonjic (4) Ivan Rungger (5) Stefano Sanvito (3)

(1) Ca' Foscari University of Venice, Italy
(2) University of Augsburg, Germany
(3) Trinity College Dublin, Ireland
(4) Institute of Physics Belgrade, Serbia
(5) UK National Physical Laboratory

Two-terminal spintronic devices remain challenging to model under realistic operating conditions, where the interplay of complex electronic structures, correlation effects and bias-driven non-equilibrium dynamics may significantly impact charge and spin transport. Existing ab initio methods either capture bias-dependent transport but neglect dynamical correlations or include correlations but are restricted to equilibrium or linear-response regimes. To overcome these limitations, we present a framework for steady-state quantum transport, combining density functional theory (DFT), the non-equilibrium Greens' function (NEGF) method, and dynamical mean-field theory (DMFT) [1,2,3,4,5]. Our framework is applicable to magnetic heterostructures such as Co/Cu/Co [3,5] and Fe/MgO/Fe [6], as well as magnetic van der Waals materials like Fe_4GeTe_2 [5], allowing for an accurate description of the spectral properties of 3d bands [6]. Furthermore, it can be extended to finite-bias conditions, beyond linear response. Our results reveal that conduction electrons can undergo bias-driven inelastic excitations [7], leading to a regime we term “hot correlated electrons” [8], which produces distinct spectral and transport signatures potentially accessible in operando experiments. More broadly, our findings uncover a general mechanism by which applied voltage reshapes electronic correlations in ferromagnetic materials.

[1] I. Rungger, A. Droghetti, and M. Stamenova, “Non-equilibrium Green’s Function Methods for Spin, Transport and Dynamics”, in Handbook of Materials Modeling: Methods: Theory and Modeling, edited by W. Andreoni and S. Yip (2020).
[2] A. Droghetti, and I. Rungger, Phys. Rev. B 95, 085131(2017).
[3] A. Droghetti, M.M. Radonjić, L. Chioncel, and I. Rungger, Phys. Rev. B 106, 075156 (2022).
[4] A. Droghetti, M.M. Radonjić, A. Halder, I. Rungger, and L. Chioncel, Phys. Rev. B 105, 115129 (2022).
[5] D. Nell, M.M. Radonjic, I., Rungger, L. Chioncel, S. Sanvito, A. Droghetti, arXiv:2511.18442
[6] D. Nell, S. Sanvito, I. Rungger, A. Droghetti, Phys. Rev. B 111, 035133 (2025).
[7] A. Halder, D. Nell, A. Sihi, A. Bajaj, S. Sanvito, and A. Droghetti, Nano Lett. 24, 9221 (2024).
[8] D Nell, S Sanvito, A Droghetti, arXiv:2510.24322

57	**Quantum interference in high harmonic generation from monolayer WS_2**	Anna Galler	Contributed talk (10:45-11:00)

Anna Galler (1) Minjeong Kim (2) Taeho Kim (2) Angel Rubio (3) Ofer Neufeld (4) Jonghwan Kim (2)

(1) TU Graz, Austria
(2) Pohang University of Science and Technology, Republic of Korea
(3) Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
(4) Technion Israel Institute of Technology

Two-dimensional hexagonal materials such as transition-metal dichalcogenides exhibit valley degrees of freedom, offering fascinating potential for valley-based optoelectronics. In nonlinear optics, the K and K’ valleys provide excitation resonances that can be used for ultrafast control of excitons, Bloch oscillations, and Floquet physics. Under intense laser fields, however, the role of coherent carrier dynamics away from the K/K’ valleys is largely unexplored. In this study, we observe quantum interferences in high harmonic generation from monolayer WS_2 as laser fields drive electrons from the valleys across the full Brillouin zone. In the perturbative regime, interband resonances at the valleys enhance high harmonic generation through multi-photon excitations. In the strong-field regime, the high harmonic spectrum is sensitively controlled by light-driven quantum interferences between the interband valley resonances and intraband currents originating from electrons occupying various points in the Brillouin zone, also away from K/K’ valleys. This joint theoretical-experimental work proposes new routes for harnessing laser-driven quantum interference in two-dimensional hexagonal systems and all-optical techniques to occupy and read-out electronic structures in the full Brillouin zone via strong-field nonlinear optics.

578	**Dynamics of electronic excitations in 1T-TaS_2**	Uwe Bovensiepen	Invited talk (11:00-11:30)

Uwe Bovensiepen (1) Kai Rossnagel (2)

(1) University of Duisburg-Essen, Faculty of Physics and CENIDE
(2) Kiel University, Institute of Experimental and Applied Physics

The transition metal dichalcogenide 1*T*-TaS_2 is known for the formation of a charge density wave with a Star-of-David shaped reconstruction of Ta atoms [1], its spin liquid behaviour [2], and its non-equilibrium hidden state [3]. The charge density wave is connected to Mott physics and formation of a Doublon excitation [4]. In this talk recent results obtained on crystals with substitutional doping using Mo and W will be presented. While both dopants decrease the degree of commensurate charge density wave order, the Star-of-David reconstruction persists. However, the electronic response is strongly modified by doping as observed in the spectral variation induced by the charge density wave amplitude mode in time-resolved photoelectron emission spectroscopy [5]. Moreover, upon doping metastable electronic excitations are identified which are populated on femtosecond timescales and persist on various timescales up to minutes which allows active switching of the local population in scanning tunnelling experiments. This work demonstrates that substitutional doping of 1*T*-TaS_2 provides manifold opportunities to manipulate local electronic excitations in solid matter.

[1] B. Sipos et al., Nat. Mater. 7, 960 (2008).
[2] M. Klanjšek et al., Nat. Phys. 13, 1130 (2017).

[3] L. Stojchevska et al., Science 344, 177 (2014).
[4] M. Ligges et al., Phys. Rev. Lett. 120, 166401 (2018).
[5] J. Jayabalan et al., arXiv:2504.19961.

164	**Mixed-configuration approximation for multiorbital systems out of equilibrium**	Tommaso Maria Mazzocchi	Contributed talk (11:30-11:45)

Markus Aichhorn (1) Enrico Arrigoni (1) Tommaso Maria Mazzocchi (1) Daniel Werner (1)

(1) Graz University of Technology

I will illustrate possible applications of the "mixed-configuration approximation" (MCA) [1,2], an approximate method that combines the solutions to independent impurity problems obtained with single-band impurity solvers to study nonequilibrium multiorbital systems at moderate computational cost. We merge the MCA with the so-called auxiliary master equation approach (AMEA) single-impurity solver. As a benchmark, I will first show that our approach reproduces the results of quantum Monte Carlo (QMC) for two-orbital impurity models at equilibrium with overall good accuracy, especially for nondegenerate orbitals. I will then use MCA+AMEA as an impurity solver for dynamical mean-field theory (DMFT) to address the case of a two-orbital, realistic layered structure, recovering the strong crystal-field-driven charge polarization observed by solving the DMFT self-consistent cycle with QMC, albeit slightly reduced. Finally, I will address a prototype nonequilibrium setup by sandwiching this layer between metallic contacts subject to a bias voltage described by different chemical potentials. This simplified model demonstrates our method's potential to access nonequilibrium steady-state behavior of multiorbital, realistic materials. These findings provide a first-step basis for theoretical studies of nonequilibrium properties of multiorbital compounds directly in the real frequency domain.

[1] Mazzocchi et al., Phys. Rev. B 112, 155127 (2025)
[2] Mazzocchi et al., arXiv:2602.05664

187	**Nonequilibrium enhancement of coherence in phase-fluctuating systems**	Duilio De Santis	Contributed talk (11:45-12:00)

Duilio De Santis (1)

(1) Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

Strong optical driving can induce transient superconducting-like behavior in materials even above their equilibrium T_c. Because many of these systems already exhibit short-range superconducting correlations in equilibrium, an important question is whether periodic driving can enhance coherence in the absence of true long-range order. To investigate this possibility, we study the two-dimensional XY model with a time-periodically modulated stiffness using overdamped Langevin dynamics. We show that, despite leaving the average coupling unchanged, the drive can significantly enhance long-range, time-averaged correlations, even at temperatures well above the equilibrium Berezinskii-Kosterlitz-Thouless transition. The response depends strongly on the competition between the drive frequency and the intrinsic relaxation rate. At high frequencies, the drive mainly acts as a source of heating, suppressing both correlations and conductivity. At lower frequencies, by contrast, the optical conductivity is reshaped: the real part exhibits an effectively longer Drude scattering time, while the imaginary part displays an enhanced low-frequency $1/\omega$ contribution. We map out these regimes as functions of temperature, drive frequency, and amplitude, and interpret them using simple analytical considerations together with a vortex-thermalization picture. Overall, our results point to a generic nonequilibrium route for enhancing coherence in XY-like systems, and we comment on its possible relevance to experiments on light-induced superconductivity in cuprates.

D. De Santis, M. H. Michael, S. Chattopadhyay, A. Cavalleri, G. Refael, P. A. Lee, E. A. Demler, “Enhanced coherence in the periodically driven two-dimensional XY model”, arXiv:2511.12287 (2025)

744	**Breaking symmetries of crystals using nonlinear phononics**	Alaska Subedi	Contributed talk (12:00-12:15)

Alaska Subedi (1)

(1) CNRS

Coherent driving of phonons with intense laser pulses usually does not lower the symmetry of a crystal. It generally causes large oscillations about the equilibrium structure or displaces the lattice along a fully symmetric coordinate. This makes it difficult to use light to reach lower-symmetry structures. I will discuss how nonlinear phononics can overcome this limitation through biquadratic couplings between two different phonon coordinates. In strained $KTaO_3$, such a coupling between zone-center modes can induce ferroelectricity. I will then show that the same idea can be extended to zone-boundary phonons, where it provides a way to break translational symmetry. In $KTaO_3$ this effect requires unrealistically high laser intensities, but it illustrates a mechanism for light-induced symmetry lowering beyond the zone center.

M03 – Session 2 (Mon 21, 16:00-18:00, Chair: Denis Golez)			
ID	Title	Speaker	Type
188	**Out-of-equilibrium intertwining via emergent pseudo-Goldstone mode**	Andras Szabo	Contributed talk (16:00-16:15)

R. Chitra (1) Andras Szabo (2)

(1) ETH Zurich
(2) Max Planck Institute for Solid State Research

Symmetry enlargement occurs in correlated systems when two degenerate ordered phases breaking different symmetries combine into a super-order parameter, transforming under an enlarged algebra. While this phenomenon is in principle accompanied by the emergence of new Goldstone modes rotating between microscopically distinct orders, the exploration of such collective excitations is often not realistic in real materials. Here, we present a controlled study based on a minimal driven-dissipative platform, in which a Bose-Einstein condensate is placed at the intersection of two optical cavities, realizing two competing copies of a Z2 symmetry-breaking superradiant phase transition, alongside an enlarged O(2)-symmetric manifold. Using periodic drives that exploit dynamical symmetry reduction, we show that the emergent Goldstone mode can be harnessed to intertwine the two superradiant sectors. Furthermore, going beyond the conventional phenomenology based on Landau orders, we show the emergence of a larger class of out-of-equilibrium intertwined phases, including intertwining of purely time-crystalline orders, as well as between Landau and time crystal orders.

36	**Towards a microscopic understanding of light-induced superconductivity in K_3C_{60}**	Michael Sentef	Invited talk (16:15-16:45)

Michael Sentef (1)

(1) University of Bremen

Light-induced superconducting-like responses have been observed in K_3C_{60} when driving withmid-infrared laser pulses [1], with a pronounced 10 THz resonance reported more recently [2]. Here we address the microscopic origin of this resonance. Using numerical calculations for a realistic model of K_3C_{60} we simulate the effect of a periodic drive on the strongly correlated system. We discuss a possible origin of the experimentally observed resonance and the relevant excitation pathway. Our results provide a microscopic explanation for the resonantly enhanced light-induced superconducting-like state in K_3C_{60} and strengthen its interpretation as being closely connected to superconducting pairing rather than to purely optical or nonthermal population effects.

[1] Mitrano et al., Nature 530 461–464 (2016).
[2] Rowe et al., Nature Physics 19, 1821–1826 (2023).
[3] Budden et al., Nature Physics 17, 611–618 (2021).
[4] J. I. Aranzadi, J. Tindall, P. Fadler, M. A. Sentef, forthcoming (2026).
We acknowledge funding by Deutsche Forschungsgemeinschaft (DFG, German ResearchFoundation)- 531215165 (Research Unit 'OPTIMAL')) and the European Union (ERC, CAVMAT,project no. 101124492).

430	**Role of pulse duration and chirality in high harmonic generation from a chiral Weyl semimetal**	Alba de las Heras	Contributed talk (16:45-17:00)

Alba de las Heras (1) Ofer Neufeld (2) Angel Rubio (1)

(1) Max Planck Institute for the Structure and Dynamics of Matter (MPSD)
(2) Technion Israel Institute of Technology

The potential of high harmonic generation (HHG) from chiral topological materials is under investigation. Our time-dependent density-functional theory (TDDFT) calculations in the prototypical chiral Weyl semimetal RhSi show two significant features [1]. On the one hand, a pulse-duration-sensitive cutoff in HHG arises from a progressive promotion of electron population to high conduction bands. The intricate band crossing network of RhSi favours excited ladder electrons, a mechanism that can substantially extend HHG to higher photon energies. Unlike typical scenarios, the strong multi-band coupling establishes the driving pulse duration as a key parameter that has not been exploited in solid-state HHG.
On the other hand, the chiral crystal structure of RhSi enables the synthesis of locally chiral near fields exhibiting an asymmetric instantaneous torsion on attosecond timescales. The concept of locally chiral light constitutes a novel paradigm for efficient enantiomer detection[2], predicting higher chiral sensitivity than circularly polarized or orbital angular momentum beams. Our TDDFT results show that a 3D chiral polarization is naturally imprinted in the attosecond electric field emerging from the chiral Weyl semimetal in the interaction with a circularly polarized driving pulse.
These theoretical findings motivate future experiments to track high-energy band crossings and in-situ attosecond locally chiral light, advancing prospects for compact extreme-ultraviolet sources, enantiomer detection and ultrafast optoelectronics.

[1] A. de las Heras, O. Neufeld & A. Rubio. Pulse-duration-sensitive high harmonics and attosecond locally-chiral light from a chiral topological Weyl semimetal. arXiv preprint: https://doi.org/10.48550/arXiv.2603.05346
[2] D. Ayuso, O. Neufeld, A. F. Ordonez, P. Decleva, G. Lerner, O. Cohen, M. Ivanov & O. Smirnova. Synthetic chiral light for efficient control of chiral light–matter interaction. Nature Photonics, 13(12), 866–871 (2019). https://doi.org/10.1038/s41566-019-0531-2

491	**Room-temperature memristive switching between charge density wave states**	Rok Venturini	Contributed talk (17:00-17:15)

Rok Venturini (1) Jože Gašperlin (2) Denis Golež (Jozef Stefan Institute) Davor Grabnar (2) Jan Lipič (2) Dragan Mihailovic (2) Matevž Rupnik (2) Yevhenii Vaskivskyi (2) Petra Šutar (2) Filip Ščepanović (2)

(1) Paul Scherrer Institute
(2) Jozef Stefan Institute

Control over the novel quantum states that emerge from non-equilibrium conditions is of both fundamental and technological importance. Metastable charge density wave (CDW) states are particularly interesting as their electrical manipulation could lead to ultra-efficient memory devices. However, using

electrical pulses for non-volatile resistance switching involving CDW states has so far been limited to cryogenic temperatures. Here, we investigate a recently discovered layered semiconductor $EuTe_4$, which exhibits the coexistence of distinct CDW orders. We report that electrical pulses can be used for excitation to non-equilibrium, yet stable electronic states across a broad temperature range from 6 K to 400 K. We find that switching occurs through a non-thermal pathway and is reversible via a thermal erase procedure. The resistance of the new electronic state is tunable by the pulse voltage, so the device acts as a memristor. Calculations show fixed bilayer CDW, whereas CDW in single layers shows bistability due to weak Eu-Te links. Low-voltage, fast, and energy-efficient CDW switching holds potential for memristor applications.

M03 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
213 **P002**	**Altermagnetic systems out of equilibrium**	Sebastian Alois Fuchs	Poster

Sebastian Alois Fuchs (1)

(1) TU Graz

Altermagnets combine collinear antiferromagnetic order with momentum-space spin splitting and anisotropic responses, offering a platform for unconventional spin and charge transport without net magnetization. We investigate nonequilibrium properties of two-dimensional altermagnetic models driven by an applied bias that sustains a steady current. Our approach is based on dynamical mean-field theory (DMFT) with the auxiliary master equation approach (AMEA) as impurity solver, enabling access to steady-state Green's functions and spectral properties beyond linear response. The lattice model incorporates antiferromagnetic order together with anisotropic next-nearest-neighbor hopping to capture the symmetry ingredients characteristic of altermagnetism. We focus on bias-dependent spectral features, spin-resolved currents, and the interplay between anisotropy and correlation effects in determining transport coefficients. The framework allows us to assess potential nonreciprocal or direction-dependent responses tied to the underlying crystalline symmetries. We will present the computational setup and discuss representative results and trends, emphasizing how nonequilibrium driving modifies the altermagnetic state and its transport signatures.

ID	Title	Presenter	Type
322 **P003**	**Nonequilibrium steady-states in Driven Mott Insulators: From Kondo Physics to Multiorbital correlations**	Enrico Arrigoni	Poster

Enrico Arrigoni (1) Daniel Werner (1) Paolo Gazzaneo (1) Tommaso Maria Mazzocchi (1)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology

I will highlight recent advances in the study of correlated Mott systems driven into nonequilibrium steady states. The analysis is based on an impurity solver that combines Keldysh Green's functions with the Lindblad formalism for open quantum systems [1], embedded within nonequilibrium Dynamical Mean-Field Theory. Recent methodological improvements including a Configuration Interaction treatment of the many body Lindblad equation combined with a linear functional interpolation [2] allow to address scaling behavior in the Kondo regime.
I will present results for nonequilibrium phenomena such as photovoltaic effects impact ionization in photoexcited Mott insulators and present a recent mixed configuration scheme to address correlated multiorbital systems and realistic material simulations out of equilibrium [3].

[1] E. Arrigoni et al., Phys. Rev. Lett. 110, 086403 (2013); A. Dorda et al., Phys. Rev. B 89 165105 (2014); A. Dorda et al., Phys. Rev. B 92, 125145 (2015)
[2] D. Werner et al., Phys. Rev. B 107, 075119 (2023); D. Werner and E. Arrigoni, PRR Letters 7, 6 (2025)
[3] T. M. Mazzocchi et al., Phys. Rev. B 15, 112, (2025); arXiv:2602.05664 (2026)

ID	Title	Presenter	Type
330 **P004**	**Extension of the iterated perturbation theory for arbitrary fillings to nonequilibrium steady states**	Tommaso Maria Mazzocchi	Poster

Tommaso Maria Mazzocchi (1)

(1) Graz University of Technology

I will present ongoing work on the extension of the iterated perturbation theory (IPT) impurity solver for arbitrary fillings to nonequilibrium steady-state problems. By merging the generalized IPT for arbitrary fillings proposed in Ref. [1] with the nonequilibrium Keldysh Green's function formalism [2], we extend the Ansatz for the electronic self-energy, in particular its Keldysh component. I will first show some equilibrium benchmarks and then address the nonequilibrium electron transport across a correlated impurity for selected fillings, temperatures and interaction strengths. The extended IPT is benchmarked against the auxiliary master equations approach (AMEA) impurity solver and shows overall good agreement in the regions where AMEA is reliable. This suggests that this extended IPT can be used as an approximate scheme to tackle nonequilibrium impurity problems and calls for a thorough investigation of other systems and observables, possibly within dynamical mean-field theory.

[1] Kajueter et al., Phys. Rev. Lett. 77, 131 (1996)
[2] Keldysh, Sov. Phys. JETP 20, 1018 (1965)

M04 - Non-Crystalline Quantum Matter

M04 – Session 1 (Mon 21, 10:30-12:30)			
ID	Title	Speaker	Type
472	**Realistic modelling of the spectral function and quasiparticle interference in moiré systems**	Peter Wahl	Invited talk (10:30-11:00)

Peter Wahl (1)

(1) University of St Andrews

Moiré systems have emerged as a highly tunable platform to study emergent electronic phenomena, enabling effectively materials-based quantum simulators. A key to microscopic understanding of the correlation physics is to unravel the electronic structure of these materials. Because of the low energy scales and flat bands with band widths on the order of a few millielectronvolts, spectroscopic characterization with ultra-high energy resolution is desirable. Quasiparticle interference imaging can provide such resolution, however is inherently difficult to interpret. I will show how using realistic simulation of quasi-particle interference from real-space tight-binding models provides predictions for the QPI in moiré materials, and will show comparison to experimental results both for graphene and TMDC heterostructures.

170	**Simulation of quasiparticle interference imaging in graphene with proximity-induced spin-orbit coupling**	Daniela Gonçalves	Contributed talk (11:00-11:15)

Daniela Gonçalves (1) Henrique Veiga (2) João Lopes (2) Aires Ferreira (1)

(1) School of Physics, Engineering and Technology, University of York
(2) Departamento de Física e Astronomia, Universidade do Porto

Within the rich landscape of 2D van der Waals heterostructures, proximitised graphene has garnered significant interest as a platform to study emergent spin-dependent phenomena. Here, we apply large-scale Chebyshev spectral methods to simulate the real-space electronic structure of atomic defects in graphene/atomically thin semiconductor heterostructures. This approach allows us to accurately map out the wavevector power spectrum of the quasiparticle interference (QPI) response, and thus determine the impact of proximity-induced Rashba and valley-Zeeman effects. Our study sheds light on the importance of Fermi surface spin-orbit textures in QPI imaging.

374	**Bulk Impurities/Vacancies in Nodal Loop Semimetals**	João Santos Silva	Contributed talk (11:15-11:30)

João Santos Silva (1) Miguel Araújo (2) Eduardo Castro (3) Vítor M. Pereira (4)

(1) CF-UM-UP, Centro de Física do Porto, FCUP
(2) Departamento de Física, Universidade de Évora
(3) Centro de Física das Universidades do Minho e Porto, LaPMET
(4) University of Porto

Weyl nodal loop semimetals are topological semimetals where the valence and conduction bands linearly touch along one dimensional loops in momentum space. A manifestation of their non-trivial topology is the presence of zero energy surface states, induced by chiral symmetry, on surfaces parallel to the loop plane. Unlike their insulator counterparts, these exotic phases may be unstable to small perturbations that respect their topology-protecting symmetries. Results for symmetry-breaking disorder have been reported. However, the case of vacancies preserves the underlying symmetry, and remains largely open. Here, we will discuss the effects of impurities and vacancies in the bulk of a nodal loop semimetal tight-binding model, as well as an effective low energy model for a circular nodal loop, where an analytical approach is tractable. We focus on the changes in the density of states (DOS), computed via a projected Green's function formalism, and study the linear optical conductivity in the presence of vacancies. We have found that a single impurity induces a peak in the DOS, which traverses zero energy as the impurity strength increases, becoming sharper near the Fermi level, in line with known literature. A single cell-vacancy creates broad peaks near the Fermi level, but the system remains a semimetal, whereas orbital vacancies induce a sharp peak at zero energy. Contrary to Weyl semimetals, we found that the nodal loop has a finite critical impurity strength that yields a finite DOS at zero energy.
The optical conductivity in the presence of site vacancies has a sharp absorption edge at $\omega = E_F$, followed by a power law decay which, for a single vacancy, goes as $\sim 1/\omega^2$. The cell vacancy case reveals a complete vanishing of the optical gap.

728	**Efficient Real-Space Simulation of Inhomogeneous Correlated Matter**	Henrique Veiga	Contributed talk (11:30-11:45)

Henrique Veiga (1,2) João Lopes (1) Aires Ferreira (2)

(1) Centro de Física das Universidades do Porto e Minho
(2) University of York

In condensed matter systems where translational invariance is inevitably or deliberately broken, probing local observables is paramount to addressing a wealth of intriguing phenomena, such as multifractality, quasiparticle interference and real-space orbital magnetic textures.
In this talk we show that the well-known computational bottleneck of computing local properties in non-periodic lattices of realistic sizes can be circumvented by the use of a novel, highly scalable real-space approach [1]. After demonstrating its significant advantages by benchmarking on the π-flux model with isolated and clustered defects, we extend our numerical framework to inhomogeneous correlated systems [2]. As a proof of concept, the method is used to investigate the local robustness of s-wave and p-wave superconducting phases in disordered graphene in a fully non-perturbative fashion. These results bring opportunities for the real-space simulation of non-periodic quantum phases of matter beyond previous approaches.

[1] Veiga, H. P., Pinheiro, D. R., Pires, J. P. Santos, & Lopes, J. M. Viana Parente. (2025). Markov Inequality as a Tool for Linear-Scaling Estimation of Local Observables. 10.48550/arxiv.2510.21688

[2] João, S. M., Viana Parente Lopes, J. M., & Ferreira, A. (2022). High-resolution real-space evaluation of the self-energy operator of disordered lattices: Gade singularity, spin–orbit effects and p-wave superconductivity. Journal of Physics: Materials, 5, 045002

316	**Real-Space Theory of Nonequilibrium Orbital Magnetization in Non-crystalline Systems**	João Manuel Alendouro Oliveira Pinho	Contributed talk (11:45-12:00)

João Manuel Alendouro Oliveira Pinho (1) Bruno Amorim (2) Aires Ferreira (3) João Lopes (1) Daniel Passos (4) Ivo Souza (4) Henrique Veiga (1) Alessandro Veneri (5)

(1) Centro de Física do Porto
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(3) School of Physics, Engineering and Technology, University of York
(4) Centro de Fisica de Materiales
(5) University of Rome Sapienza

The nonequilibrium generation of orbital magnetization under applied electric fields is a central problem in the emergent field of orbitronics. However, its theoretical description is challenging due to the ill-defined nature of the position operator under periodic boundary conditions. While the modern theory of orbital magnetization reformulates the problem in the Bloch representation, its generalization beyond equilibrium and the perfect (clean) crystal limit is yet to be fully developed. Here, we present a general-purpose real-space approach to nonequilibrium orbital magnetization, which does not rely on the position operator, and that can be applied to systems that do not exhibit perfect translational invariance, including disordered and quasiperiodic materials. The utility of the new formalism is demonstrated by numerical tight-binding studies of the orbital Edelstein effect in the disordered Haldane model.

511	**Band structures of hyperbolic tight-binding models: Leveraging the HyperCells and HyperBloch software packages**	Tomáš Bzdušek	Contributed talk (12:00-12:15)

Marcelo Looser (1) Mykhailo Pavliuk (1) Joseph Maciejko (2) Tomáš Bzdušek (1) Patrick M. Lenggenhager (3)

(1) University of Zurich
(2) University of Alberta, Edmonton
(3) Max Planck Institute for the Physics of Complex Systems, Dresden

Hyperbolic lattices constitute synthetic matter in which sites are more densely interconnected than in ordinary lattices, leading to an effective negative curvature at large length scales. Such systems have in recent years been successfully realized across a range of experimental platforms, including coupled microwave resonators, electric-circuit networks, and silicon photonics. This experimental progress has also fueled theoretical efforts to characterize models on hyperbolic lattices, which notably include a non-Abelian generalization of the Bloch theorem with infinite-dimensional reciprocal space [1,2,3].
In Ref. [4], we introduced an approximate numerical scheme rooted in computational group theory, the hyperbolic supercell method, which enables a controlled and convergent treatment of these generalized Bloch states. We have since implemented this scheme in a pair of tandem software packages: HyperCells and HyperBloch. In this contribution, I will present excerpts from an upcoming work [5] that demonstrates the efficiency and the broad applicability of the supercell method across a diverse set of hyperbolic lattice models, including systems with topological and flat energy bands, mean-field-treated density waves in hyperbolic Hubbard models, and quantum spin liquids in hyperbolic Kitaev models.

[1] J. Maciejko and S. Rayan, Automorphic Bloch theorems for hyperbolic lattices, Proc. Natl. Acad. Sci. U.S.A. 119, e2116869119 (2022).
[2] N. Cheng, F. Serafin, J. McInerney, Z. Rocklin, K. Sun, and X. Mao, Band Theory and Boundary Modes of High-Dimensional Representations of Infinite Hyperbolic Lattices, Phys. Rev. Lett. 129, 088002 (2022).
[3] G. Shankar and J. Maciejko, Hyperbolic Lattices and Two-Dimensional Yang-Mills Theory, Phys. Rev. Lett. 133, 146601 (2024).
[4] P. M. Lenggenhager, J. Maciejko, and T. Bzdušek, Non-Abelian Hyperbolic Band Theory from Supercells, Phys. Rev. Lett. 131, 226401 (2023).
[5] M. Looser, M. Pavliuk, J. Maciejko, T. Bzdušek, and P. M. Lenggenhager, Band structures of hyperbolic tight-binding models: Leveraging the HyperCells and HyperBloch software packages (in preparation, 2026).

212	**Topological Gyromorphs**	Isidora Araya Day	Invited talk (12:15-12:45)

Isidora Araya Day (1) Adam Chaou (1) Adolfo Grushin (1) Laura Gómez Paz (2) Justin Schirmann (2)

(1) DIPC
(2) CNRS

Gyromorphs are a new class of disordered systems that combine an amorphous-like absence of translational order with quasi-long-range rotational order. Gyromorphs can outperform quasicrystals or hyperuniform arrangements in forming isotropic band gaps, suggesting an avenue to realize robust disordered topological phases. However, gyromorphs lack exact rotational symmetry, which is only realized on average, posing an obstacle for existing real-space invariants to correctly diagnose topological gyromorphs.
In this talk I will show that gyromorphs can host higher-order topological insulating (HOTI) phases protected by average rotational symmetry, and discuss the tools for diagnosing topological phases protected by such symmetry. I will show that symmetry indicators of the effective Hamiltonian, the spectral localizer, and scattering invariants all draw a consistent topological phase diagram.

M04 – Session 2 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
140	**Universal mechanism for ferromagnetism in localized quasiperiodic moiré systems**	Miguel Gonçalves	Invited talk (16:00-16:30

Miguel Gonçalves (1) Sarang Gopalakrishnan (2)

(1) Princeton Center for Theoretical Science, Princeton University
(2) Department of Electrical and Computer Engineering, Princeton University, Princeton NJ 08544, USA

We unveil a mechanism for ferromagnetism in quasiperiodic moiré systems hosting a narrow band of localized states. By projecting the full interacting Hamiltonian onto the narrow band, we numerically and analytically determine the stability of the fully polarized ferromagnetic state at half filling of the narrow band against charge and spin-flip excitations, converging the results to the thermodynamic limit in both 1D and 2D.
Our analytical theory shows that the geometry of single-particle eigenstate overlaps governs magnon excitations and the stability of the ferromagnet.
Under certain off-resonant conditions for the single-particle eigenstates, the critical interaction strength for ferromagnetism can become much smaller than the energy gap to remote bands, a regime where our projected theory becomes asymptotically exact.
We contrast our result with the celebrated Lieb theorem for half-filled Hubbard models on bipartite lattices - where a fully-polarized ferromagnetic ground state is forbidden for any repulsive interaction strength - and show how weakly breaking bipartiteness can stabilize ferromagnetism at small interaction strengths in our setup.

512	**Signatures of Incommensurability in moiré Quasicrystals**	Raul Liquito	Contributed talk (16:30-16:45)

Raul Liquito (1)

(1) Faculdade de Ciências da Universidade do Porto - Departamento de Física e Astronomia, CF-UM-UP

Moiré materials represent one of the richest fields in condensed matter physics, with twisted bilayer graphene (TBG) serving as a prime example. TBG exhibits exotic physical properties, including unconventional superconductivity and delocalized eigenstates in both momentum and real space near the flat-band regime. Recent experiments on hBN/TBG and twisted trilayer graphene (TTG) have uncovered a new, intrinsically quasiperiodic regime driven by competing incommensurate moirés, dubbed moiré quasicrystals. Because these phases also host robust correlated states, understanding the exact role of quasiperiodicity is essential to determine whether such phenomena are driven by correlation, topology, or the explicit breaking of translational invariance.
To address this, we perform real-space atomistic tight-binding simulations of 2D moiré materials containing up to 10 million atoms. By comparing quasiperiodic and commensurate (unit cell = 1 moiré cell) TBG, we conduct a multifractal analysis of the local density of states to extract the singularity spectrum, a quantity directly accessible to experimentalists via STS maps. Our results show that incommensurate magic-angle TBG, the flat band is strictly multifractal, whereas commensurate structures remain monofractal. In contrast, the remote bands exhibit perfect monofractal behavior across both regimes.

397	**Quantics Purification Mean-field approach to 2D moiré materials**	Nicolau Sobrosa	Contributed talk (16:45-17:00)

Nicolau Sobrosa (1) Bruno Amorim (1) Tiago Antão (2) Eduardo Castro (1) Jose Lado (2) Pedro Ribeiro (3) Yitao Sun (2)

(1) University of Porto
(2) Aalto University
(3) Instituto Superior Técnico

The emergence of correlated phases, such as unconventional superconductivity, in two-dimensional moiré materials is one of the most fascinating developments in condensed matter physics. However, the interplay between the large-scale moiré patterns, the formation of flat bands, and the subsequent interaction-induced phases poses a significant challenge for numerical simulations. In realistic settings, twist-angle disorder or substrate interactions are sufficient to break translation symmetry or create super-moiré effects precluding the use of standard continuum models.
To overcome this, we propose a mean-field approach enhanced by quantics tensor networks. By utilizing a tensor-train representation of the mean-field Hamiltonian and the reduced density matrix, this method achieves logarithmic scaling with the system size. This scaling is a crucial advantage, enabling the simulation of exponentially large systems and capturing super-moiré physics. By comparison, exact diagonalization or even linear scaling methods such as the Fermi Operator Expansion become prohibitive at this length scales.
In this work, we study a two-dimensional model hosting both flat bands and incommensurability-induced critical states. We introduce a zero-temperature purification scheme of the reduced density matrix that takes the tensor-network representation of the mean-field Hamiltonian and iteratively applies a low-order polynomial, converging to the density matrix.
We analyze the real-space distribution of the charge density as well as its Fourier transform, to detect the presence of quasi-fractal order. Finally, we will discuss the physical implications of this quasi-fractal order for the broader understanding of strongly correlated phases in super-moiré systems.

285	**Tensor network approach to real-space superconductivity in quasicrystals**	Ricardo Oliveira	Contributed talk (17:00-17:15)

Ricardo Oliveira (1) Bruno Amorim (1) Tiago Antão (2) Eduardo Castro (1) Jose Lado (2) Yitao Sun (2)

(1) Centro de Física das Universidades do Minho e Porto, LaPMET
(2) Department of Applied Physics, Aalto University

The recent discovery of superconductivity in quasiperiodic twisted trilayer graphene (tTLG) underscores the complex interplay between quasiperiodicity and interactions in moiré materials [1]. Furthermore, previous work by the authors [2] has shown that quasiperiodicity can lead to an enhancement of superconductivity in one-dimensional quasiperiodic models. However, a proper theoretical description of superconductivity in quasiperiodic moiré materials is still lacking, due to the lack of translational invariance that implies that real-space numerical methods must be necessarily employed to study moiré systems such as twisted bilayer graphene (tBLG), requiring the simulation of system sizes in the order of millions of atoms [3].

We propose a real-space tensor network approach to study s-wave superconductivity in two-dimensional quasicrystals with eightfold rotational symmetry. Building on the tensor network kernel polynomial method combined with the quantics tensor cross interpolation method (QTCI) to represent ultra-large real-space Hamiltonians [4, 5], we can obtain real-space mean-field solutions for on-site pairing across systems exceeding one million sites. This scalable approach enables computation of the local density of states and the spatially resolved superconducting pairing, revealing how eightfold symmetry and the quasiperiodic structure of the system shapes the texture of s-wave order. Our work opens a path towards quantitative real-space characterization of superconductivity in quasiperiodic moiré systems that require large-scale simulations.

[1] A. Uri et al., Nature 620 (2023) 762–767
[2] R. Oliveira et al., arXiv preprint (2023) 2303.17656
[3] Miguel Gonçalves et al., 2D Mater 9 (2021) 011001
[4] Yitao Sun et al., arXiv preprint (2025) 2503.04373
[5] Tiago V. C. Antão et al., arXiv preprint (2025) 2506.05230

54	**Number theory meets physics: the curious case of the Aubry-André model**	Balázs Hetényi	Contributed talk (17:15-17:30)

Balázs Hetényi (1)

(1) Budapest University of Technology and Economics

One of the most frequently cited experimental results in condensed matter physics are those of the quantum Hall effect. These results show peaks in the Hall conductance as a function of magnetic flux at rational numbers of elementary flux units, implying that the experiment distinguishes between rational and irrational flux. In this talk I will present results for the Aubry-André model, a model which is equivalent to the Harper model (used to understand the quantum Hall effect). We study the model as a function of particle density and find that sharp peaks (spikes) occur in the localization-delocalization phase diagram: at rational fillings the transition occurs at a finite potential strength, while at certain accessible irrational fillings, the system is always localized (the transition occurs at zero potential strength). Our studies use extensions of the modern theory of polarization which casts the polarization as a geometric phase, rather than an operator expectation value. We have developed the analog of the Binder cumulant for geometric phases. To explain the presence of spikes, we invoke the Zeckendorf decomposition of natural numbers as an explanation. Time permitting we will connect our results to those of the quantum Hall effect.

B. Bánfalvi and B. Hetényi, work in progress.
B. Hetényi and I. Balogh, Phys. Rev. B 112 144203 (2025).
B. Hetényi, Phys. Rev. B 110 125124 (2024).

166	**Quantum geometry in disordered and quasicrystalline matter**	Annica Black-Schaffer	Invited talk (17:30-18:00)

Annica Black-Schaffer (1)

(1) Uppsala University

Quantum geometry provides a unifying framework to describe wave-function structure. In this talk, I introduce the quantum metric as a natural tool to characterize non-crystalline quantum matter, as it captures both impurity correlations and localization.
In graphene with vacancy disorder, where defect states form a zero-energy impurity band with multifractal character, a spatially resolved quantum metric reveals strongly enhanced correlations arising from long-range coupling between vacancies. In Fibonacci quasicrystals, the quantum metric likewise characterizes localization by incorporating distances between local symmetry centers. At the same time, the full quantum geometry directly links the localization properties to the fractal energy spectrum.

M05 - Transport in Low-Dimensional Strongly Correlated Quantum Systems

M05 – Session 1 (Wed 23, 10:30-12:30, Chair: Igor Yurkevich)			
ID	Title	Speaker	Type
88	**Variety of fractional conductances and fractional charges in the strongly interacting one-dimensional systems**	Victor Kagalovsky	Invited talk (10:30-11:00)

Victor Kagalovsky (1)

(1) Shamoon College of Engineering

This research considers a strongly interacting one-dimensional system with N channels and explains the variety of experimentally observed fractional conductances in GaAs/AlGaAs heterostructures [1-3]. We study relevant backscattering perturbations that create gaps in the corresponding fields, thereby altering the system's properties. We model these gapped fields by introducing masses for the bosonic fields and sending them to infinity to compute the correlator of the two fields that describe the original channels. The exact solution of the corresponding Green function in the low-frequency limit enables us to apply the Kubo formula to calculate the system's dc conductance [4], which accounts for all the seminal experimental results [1-3]. We construct a pseudo-orthogonal transformation that reduces each backscattering term to a single-channel field [5] and derive the expression for the fractional charge transferred during the tunneling of the gapped mode, which dominates the dc shot noise. The coexistence of two gapped modes (two relevant perturbations) affects the tunneling of fractional charges in each of the modes.

[1] Y. Gul, S. N. Holmes, M. Myronov, S. Kumar, M. Pepper, J. Phys. Condens. Matter 30, 09LT01 (2018)
[2] S. Kumar, M. Pepper, S. N. Holmes, H. Montagu, Y. Gul, D. A. Ritchie, I. Farrer, Phys.Rev. Lett. 122, 086803 (2019)
[3] S. Kumar, M. Pepper, Appl. Phys. Lett. 119, 110502 (2019).
[4] R. Davies, V. Kagalovsky, and Igor. V. Yurkevich, Low Temperature Physics 52, (2026).
[5] R. Davies, V. Kagalovsky, and Igor. V. Yurkevich, Crystals 15, 818 (2025).

112	**Reconstructive phase transitions in a-GeSbTe and a-GeTe compounds**	Zvi Ovadyahu	Invited talk (11:00-11:30)

Zvi Ovadyahu (1)

(1) Racah Institute of Physics, The Hebrew University Jerusalem ISRAEL

Films of amorphous GeSbTe and GeTe exhibit nonequilibrium transport anomalies when subjected to thermal cycling. These presumably reflect iso-thermal structural changes. Some of these temperature-driven changes are reversible, suggestive of a phase-transition occurring at the amorphous phase. Noise measurements are consistent with this picture while revealing a qualitative difference between the two compounds.

249	**Tailoring Quantum States in Oxide-Based Memristive Nanodevices: From Strong Correlations to Neuromorphic Computing**	Victor Rouco	Invited talk (11:30-12:00)

Victor Rouco (1) S.J. Carreira (2) V. Humbert (3) A. Lagarrigue (3) C. Leon (1) G. Sanchez-Santolino (1) J. Santamaria (1) Z. Sefrioui (1) I. Tenreiro (1) M. Varela (1) J.E. Villegas (3) V. Zamora (1) C. de Dios (1)

(1) Universidad Complutense de Madrid (UCM)
(2) Unité Mixte de Physique CNRS/Thales
(3) Laboratoire Albert Fert, CNRS, Thales, Université Paris Saclay

Complex oxide materials stand at the forefront of solid-state quantum technologies, offering a rich playground where quantum properties can be finely tuned via external stimuli. The interplay between competing ground states in these systems not only unveils fascinating fundamental physics but also paves the way for multifunctional applications. Among these, oxide-based tunnel junctions have emerged as one of the leading candidates for the next generation of memristors: the building blocks of energy-efficient neuromorphic computing architectures.
In this talk, I will showcase our recent breakthroughs in oxide memristive devices, shifting the focus toward novel freestanding architectures and transport characterization, including light illumination. We will explore how a deterministic manipulation of quantum states at the nanoscale can be achieved across diverse functionalities—such as ferroelectricity, ferromagnetism, and superconductivity. By harnessing these strongly correlated phases, we demonstrate control over the device's response, bridging the gap between fundamental quantum phenomena and the future of solid-state nanodevices.

482	**Emergent Hall viscosity in the integer quantum Hall phases of graphene-like systems**	Maik Selch	Contributed talk (12:00-12:15)

Maik Selch (1) Mikhail Zubkov (1)

(1) Ariel University

We introduce the concept of emergent Hall viscosity in condensed matter systems whose effective field theories incorporate strain-induced emergent vielbein, metric, and gauge fields. This framework provides a unified description of previously studied contributions, which we term electronic and geometric Hall viscosities, and naturally allows for additional mixed terms. As a concrete example, we analyze graphene-like systems subjected to a magnetic field in the integer quantum Hall regime as well as the non-relativistic limit of their Semenoff-type massive semiconducting phase. We present a Green function representation of the emergent Hall viscosity and examine its topological robustness. Within this setting, we propose an experimental protocol based on twisted bilayer graphene to disentangle the different viscosity contributions.

359	**Interband spin-orbit coupling effect on chirality-induced spin-polarized current**	Misa Nozaki	Contributed talk (12:15-12:30)

Misa Nozaki (1) Takatoshi Fujita (1)

(1) National Institutes for Quantum Science and Technology

Chirality-induced spin selectivity (CISS), in which electrons transmitted through nonmagnetic chiral materials exhibit strong spin-dependent transport, has attracted growing interest for spintronic applications [1]. Experiments have reported spin polarizations of several tens of percent in a variety of quasi-one-dimensional chiral systems, including DNA, oligopeptides, helicenes, and helical molecular aggregates. Although theoretical mechanisms based on intraband spin–orbit coupling (SOC) and on-site Coulomb interactions have been proposed [2,3], a quantitative understanding of CISS remains elusive, partly because most previous studies rely on single-band models.
In this work, we theoretically investigate multiband effects on the magnetoresistive response associated with CISS. We adopt a two-site, two-band extended Hubbard model as a minimal model for chiral molecular aggregates, incorporating interband SOC, on-site Coulomb interactions, and electron hopping. The nonequilibrium steady-state current is evaluated using the Gorini–Kossakowski–Lindblad–Sudarshan (GKLS) master equation.
We show that the magnetoresistive effect vanishes in the absence of electron correlations, whereas finite Coulomb interactions induce a sizable spin polarization that is enhanced with increasing interaction strength. Notably, spin polarization exceeding 25% is achieved even when the SOC strength is much smaller than the electron hopping amplitude. These results demonstrate the essential role of interband SOC in multiband CISS mechanisms.

[1] D. H. Waldeck, R. Naaman, and J. Subotnik, Physics Today (2026).
[2] J. Fransson, J. Phys. Chem. Lett. 10, 7126 (2019).
[3] K. H. Huisman et al., J. Phys. Chem. C 127, 6900 (2023).

M05 – Session 2 (Wed 23, 16:00-18:00, Chair: Igor Yurkevich)

ID	Title	Speaker	Type
293	**Extended hot-electron model and current bistability in insulating α-Y_xSi_{1-x} films**	Miguel Ortuño	Invited talk (16:00-16:30)

Miguel Ortuño Ortín (1) Le Hong Hoang To (2) Claire Marrache-Kikuchi (2) Andrés Somoza (1)

(1) Universidad de Murcia
(2) Université Paris-Saclay, CNRS, IJCLab

This work investigates bistable current-voltage (I–V) characteristics in amorphous a-YxSi1−x thin films, where disorder is controlled by thermal annealing. When a disordered insulator is biased electrically, the electron system can heat up well above the phonon bath temperature due to weak electron-phonon coupling, giving rise to multiple non-equilibrium steady states and abrupt jumps of up to four orders of magnitude in current. Experiments were carried out in a dilution refrigerator down to 13 mK, allowing the identification of the critical disorder level at which bistability first emerges and the characterization of the associated hysteresis in the nonlinear I–V curves.
To interpret these results, the authors first provide a microscopic derivation of the phenomenological hot-electron model, grounding it in the physics of electron hops between metallic-like grains embedded in an insulating matrix. In this picture, Coulomb interactions enable fast phononless thermalization across the sample, justifying a single well-defined electronic temperature Teff, while energy relaxation is governed by intra-grain electron-phonon transitions scaling as P ∝ α(Teff^β − Tph^β) with β = 6.
For the more insulating samples (annealed at 95 °C), this standard hot-electron model provides excellent quantitative agreement with experiment. However, for samples with lower disorder (80 °C), significant discrepancies arise, motivating two extensions: (i) incorporation of electric field-assisted hopping, which lowers the effective activation energy in a field-dependent resistance, and (ii) phonon-mediated inter-grain charge transfer, which introduces an additional relaxation channel that becomes dominant at high voltages. The extended model reproduces the experimental I–V curves across all disorder regimes, with fitting parameters fully consistent with the linear-response data.

559	**Electron-phonon decoupling in disordered films**	Igor Lerner	Invited talk (16:30-17:00)

Igor Lerner (1) George McArdle (2)

(1) School of Physics, University of Birmingham, UK
(2) University of Nottingham

Tremendous experimental progress in ultracold atomic systems, isolated from the environment, led to the observation of many-body localization (MBL). The question remains, however, whether MBL can be observed in disordered electronic systems for which it was originally predicted. For this, decoupling from the lattice phonons is required, which is possible only in out-of-equilibrium systems. Here I show that in suspended films such an electron-phonon decoupling may happen, manifesting itself via a bistability in the electron temperature which can be observed experimentally through hysteretic jumps of several orders of magnitude in the nonlinear current-voltage characteristics. A necessary condition for such a regime is an Arrhenius form of the equilibrium conductivity. I report on experiments with suspended films where the bistability has been observed.

345	**Thermalization in two-dimensional strongly correlated quantum systems**	Dragana Popovic	Invited talk (17:00-17:30)

Dragana Popovic (1)

(1) National High Magnetic Field Laboratory, Florida State University

The mechanisms that quantum systems can use to avoid thermalization and retain information in their local degrees of freedom have been a subject of intense research interest for both new fundamental physics and novel applications. These mechanisms, for example, are of great importance for quantum technologies since they can be used to build quantum memory devices. This talk will discuss transport measurements that probe the approach to thermal equilibrium in an open two-dimensional electron system at different densities across the metal-insulator transition. We observe different types of far-from-equilibrium dynamics, including many-body localization (MBL). We establish the phase diagram of the dynamical behavior that shows the crossover between MBL and ergodic regimes as a function of density and bath temperature.

331	**Towards an automated discovery of advanced topological insulators operating at elevated temperatures**	Oleg Yevtushenko	Invited talk (17:30-18:00)

Oleg Yevtushenko (1) Herbert Maczko (1) Stefan Birner (1)

(1) nextnano GmbH

After the seminal discovery of two-dimensional (2D) topological insulators (TIs) in CdTe/HgTe single-layer quantum wells (QWs), these fascinating systems have emerged as promising candidates for various devices in topological electronics and spintronics. One of the key limiting factors for practical applications of TIs is a small band gap, which results in low operating temperatures, usually not exceeding 15 K for CdTe/HgTe QWs. Hence, the search for application-suitable alternatives is in high demand.
One possible direction is provided by InAs/Ga_{1−x}In_{x}Sb bilayer QWs. Perhaps the most promising results have recently been obtained in InAs/Ga_{0.65}In_{0.35}Sb/InAs triple QWs, where stable helical edge transport has been observed at temperatures up to 60 K. Importantly, the geometry of 2D TIs operating at elevated temperatures is becoming increasingly complex. As a result, the design space – material composition, layer thicknesses, etc. - becomes high-dimensional and strongly nonlinear. This makes conventional trial-and-error approaches impractical and motivates the need for automated discovery strategies.
In this talk, we will discuss how two modern automated approaches - Evolutionary Algorithms and Machine Learning (specifically Reinforcement Learning) - can be applied to the search for advanced topological insulators based on quantum well heterostructures. We will outline the advantages and disadvantages of these strategies. Focusing on the example of a triple quantum well, we will demonstrate how the combination of advanced numerical tools with Evolutionary Algorithms can accelerate the discovery of optimized structures for advanced TIs.

M05 – Session 3 (Fri 25, 10:30-12:30, Chair: Wolfgang Lang)

ID	Title	Speaker	Type
550	**Giant photoconductance via an optically induced 2DEG at correlated oxide interfaces**	Javier E. Villegas	Invited talk (10:30-11:00)

D. Sanchez-Manzano (1) G. Krieger (2) A. Raji (2) B. Geisler (3) V. Humbert (1) H. Jaffres (1) J. Santamaria (4) R. Pentcheva (3) A. Gloter (5) D. Preziosi (2) Javier E. Villegas (1)

(1) Laboratoire Albert Fert, CNRS, Thales, Université Paris-Saclay, France
(2) Institute of Physics and Chemistry of Materials of Strasbourg, CNRS, University of Strasbourg, France
(3) Department of Physics and Center for Nanointegration (CENIDE), University of Duisburg-Essen, Germany
(4) Departamento de Física de Materiales, Universidad Complutense de Madrid, Spain
(5) Laboratoire de Physique de Solides, CNRS, Université Paris-Saclay, France

We demonstrate, through experiments (transport, electron microscopy & spectroscopy) and density functional theory (DFT), that a high mobility 2DEG can be optically switched on and off at a correlated oxides interface where such an electronic state does not naturally exist [1]. In particular, we find that near-ultraviolet light instantly creates a volatile 2DEG at the interface between SrTiO3 (a band insulator) and infinite-layer NdNiO2 (a poor metal), resulting in a conductivity increase of up to five orders of magnitude. This dramatic stems from structural and electronic reconstruction that, along with a built-in interfacial electric field, facilitates the Ti-3d band occupation by photogenerated carriers. These findings open avenues for engineering photoconductance in strongly correlated systems.

498	**Absolute measurement of penetration depth of superconducting thin films using microwave stripline resonators**	Pratap Raychaudhuri	Invited talk (11:00-11:30)

Arghya Dutta (1) Sulagna Dutta (1) Pratap Raychaudhuri (1) Ajit Salunke (1)

(1) Tata Institute of Fundamental Research, Mumbai

Superconducting microstrip resonators, which leverage kinetic inductance to probe electrodynamics, are sensitive tools for studying superconducting thin films at microwave frequencies. However, extracting the absolute superconducting penetration depth from these measurements remains challenging. In this talk, I will present a hybrid method to determine the absolute value of over a wide temperature range by combining resonator measurements with finite-element electromagnetic simulations in COMSOL Multiphysics. We demonstrate this approach by extracting the penetration depth of NbN films by fabricating resonators from films of various thicknesses. Furthermore, we extend the technique to materials with lower critical temperatures by employing a flip-film geometry. By placing a sample above a NbN resonator, separated by a thin Mylar dielectric, we create a coupled structure where changes in the sample's penetration depth shift the resonant frequency. This non-destructive method provides a reliable, high-sensitivity platform for characterizing the penetration depth of diverse superconducting thin films. Finally, I will show the application of this technique on NiBi3, an anisotropic s-wave superconductor in the very strong coupling limit.

180	**Stabilization of relaxation and reduction of decoherence by periodic biasing of TLSs in superconducting qubit circuits**	Moshe Schechter	Invited talk (11:30-12:00)

Jose Este Jaloveckas (1) Shlomi Matityahu (2) Moshe Schechter (3) Alexander Shnirman (1)

(1) Karlsruhe Institute of Technology

(2) Quantum Machines
(3) Ben Gurion University

Structural tunneling two-level systems (TLSs), generically present in amorphous solids and at interfaces, are dominant source of noise and decoherence in quantum devices. Mitigation of their deleterious effects is thus of utmost importance in the quest of improving performance of superconducting resonators and qubits. Here I will discuss the effect of periodic biasing of the TLSs in stabilizing qubit relaxation rates and in reducing qubit decoherence rates in general, and specifically for the case of dual rail qubits.

[1] S. Matityahu, A. Shnirman, M. Schechter, Phys. Rev. Applied 16, 044036 (2021).
[2] S. Matityahu, A. Shnirman, M. Schechter, Phys. Rev. Applied 21, 044055 (2024).
[3] J. E. Jaloveckas, A. Shnirman, M. Schechter, in preparation.

237	**Long-Range Hopping in Quantum Bosons: From Non-BKT Criticality to Excitonic Supersolids**	Tanul Gupta	Contributed talk (12:00-12:15)

Tanul Gupta (1) Nikolay Prokofiev (2) Guido Pupillo (1)

(1) CESQ, University of Strasbourg
(2) UMass, Amherst

We present exact large-scale Quantum Monte Carlo results for the one-dimensional Bose–Hubbard model with power-law hopping ∼ 1/r^α. For all 1 < α ≤ 3, we find that the superfluid–Mott-insulator transition at unit filling is continuous and scale invariant, and therefore incompatible with the Berezinskii–Kosterlitz–Thouless scenario recovered only for α > 3. We characterize this new universality class through finite-size scaling, data-collapse analysis, and a study of the excitation spectrum. Long-range hopping is also shown to qualitatively reshape the superfluid phase, yielding true long-range order for α ≤ 2 and an anomalous quasi-long-range-order regime for 2 < α ≤ 3. These results establish long-range hopping as a route to unconventional criticality in one-dimensional bosonic systems. We also briefly connect these ideas to collaborative numerical work on dipolar excitons in a lattice, where long-range hopping together with dipolar interactions supports excitonic supersolid behavior at fractional fillings.

221	**Cooper quartets in interacting nonlocal Josephson junctions**	Peihao FU	Contributed talk (12:15-12:30)

Peihao Fu (1) Luca Chirolli (1)

(1) University of Florence

Beyond the concept of Cooper pairs, Cooper quartets are exotic fermionic aggregates forming the basis of charge-4*e* superconductivity. They provide a platform to explore genuine four-body interactions, with potential relevance for topological matter and strongly correlated quantum systems. However, their realization, engineering, and unambiguous detection remain outstanding challenges.
Here, we propose a scheme to realize Cooper quartets in a triple-quantum-dot system coupled to three conventional superconducting leads via a nonlocal Josephson junction. By engineering both interdot and intradot interactions, we demonstrate that the ground state can be driven into a coherent superposition of the vacuum |0> and a four-electron state |4e>, characteristic of a quartet condensate. We show that crossed Andreev reflection processes play a central role, enabling the splitting of Cooper quartets in superconductors across different quantum dots. The system is shown to support a pi-periodic Josephson current, which can be nonlocally controlled by the superconducting phase of a separate terminal.
This mechanism establishes a route to generating coherent four-body correlations in hybrid superconducting nanostructures. More generally, the nonlocal nature of the quartet ground state suggests the emergence of correlated behavior in multiterminal geometries, defining a broader class of interacting Andreev matter, potentially exhibiting nontrivial topological properties.

L. Chirolli, A. Braggio, and F. Giazotto, Cooper quartets in interacting hybrid superconducting systems, Phys. Rev. Res. 6, 033171 (2024).

M05 – Session 4 (Thu 24, 10:30-12:30, Chair: Claire Marakke-Kikuchi)

ID	Title	Speaker	Type
139	**Electric-field-driven dissipative structures in superconductors**	Shamashis Sengupta	Invited talk (10:30-11:00)

Shamashis Sengupta (1)

(1) IJCLAB (Paris-Saclay)

The problem of dissipation in superconductors is associated with variations in time of the order parameter. In low-dimensions, the appearance of a finite voltage is related to the ac Josephson effect. It may lead to the observation of a charge current consisting simultaneously of superconducting and dissipative components. A notable example of such a phenomenon is the occurrence of phase slips in quasi-one-dimensional (quasi-1D) nanowires. We will present the results of our experiments on the current-voltage characteristics of superconducting films, in which finite voltages were applied along the length. These measurements reveal the existence of an electric-field-driven intermediate state. Its key feature is the propagation of a charge current with both zero-resistance and dissipative components. The electric field is found to penetrate over large distances of few hundred micrometres while signatures of superconductivity still persist. This provides a solid-state platform for probing the physics of nonequilibrium structures in a charged quantum fluid. We will discuss how the observations vary across quasi-1D and 3D specimens.

793	**Electronic Conduction in 1D -the 0.7 and Fractions in the 1D-2D Transition**	Mike Pepper	Invited talk (11:00-11:30)

Michael Pepper (1)

(1) University College London

Confinement of a 2D electron gas to form a 1D system allows observation of conductance quantization with values of 2ne2/h where the integer n is 1,2,3,4 and the factor of 2 is spin degeneracy. This formula is based on spatial quantization and ballistic conduction. However, in 1996 a deviation from this simple behaviour occurred when a conductance plateau, or structure, was found near 0.7(2ne2/h) taking the name 0.7 structure. It is often a conductance plateau and can be between 0.8 and 0.6, the initial description of the effect was attributed to spin polarization arising from a ferromagnetic coupling, which resulted in only one spin direction being transmitted in a longer sample, with partial transmission of the other spin in a shorter sample. It is found that the conductance below the 0.7 is spin polarised. Both thermal and noise measurements indicate that the spins split with only one fully transmitted, application of a magnetic field which lifts the spin degeneracy of the plateaus also reduces the 0.7 to 0.5, ie a complete spin polarisation. It has been suggested that the spins are polarised but the polarisation axis slowly rotates in time which is consistent with the experiments.
When the confinement is weakened the 0.7 disappears, as do the first integer plateaus, and can be replaced by a new quantization with fractional values such as 1/6, ½, 1/5 and 2/5 in units of e2/h. This Non-Magnetic Fractional Quantization may be thought to have certain similarities to the Fractional Quantum Hall Effect except that there is no magnetic field, the fractions can be even as well as odd and there is no filling factor to determine the fractional value. This effect has been found in a range of semiconductors such as electrons in GaAs, InGaAs, InAs and holes in GaAs. These effects will be discussed along with possible theoretical explanations.

108	**Collective depinning and sliding of a quantum Wigner crystal in a two-dimensional electron system**	Sergey Kravchenko	Invited talk (11:30-12:00)

Sergey Kravchenko (1) Michael Melnikov (2) Alexander Shashkin (2)

(1) Physics Department, Northeastern University
(2) Institute of Solid State Physics, Chernogolovka

We will report the observation of two-threshold voltage-current characteristics accompanied by a peak of broadband noise between the two threshold voltages, V1 and V2, in the insulating state at low electron densities in two-dimensional electron systems in silicon metal-oxide-semiconductor field-effect transistors and ultrahigh mobility SiGe/Si/SiGe heterostructures. These two-threshold V – I characteristics are strikingly similar to the two-threshold I – V characteristics known for the collective depinning of the vortex lattice in type-II superconductors, with voltage and current axes interchanged. The observed results can be described by a phenomenological theory of the collective depinning of elastic structures, which naturally generates a peak in broadband current noise between the dynamic (Vd) and static (Vs) thresholds and changes the crystal's sliding over a pinning barrier above the static threshold. This provides compelling evidence for the formation of a Wigner crystal in these structures and demonstrates the generality of the effect across different classes of strongly correlated two-dimensional electron systems.

M05 – Session 5 (Thu 24, 16:00-18:00, Chair: Vincent Humbert)

ID	Title	Speaker	Type
75	**Superconducting Diodes Enabled by Correlated Flux Quanta Dynamics**	Oleksandr Dobrovolskiy	Invited talk (16:00-16:30)

Oleksandr Dobrovolskiy (1)
(1) Technische Universität Braunschweig

Studies of rectified transport in systems lacking reflection symmetry (ratchets) have been a subject of sustained interest for many decades [1]. In recent years, the superconducting diode effect has attracted considerable attention, both for enabling rectification without Joule heating in low-power electronics and as a manifestation of broken reciprocity in coherent quantum condensates [2,3]. In this talk, I will present our recent results on nonreciprocal transport in superconductor-based systems, achieved through the engineering of edge barriers [4] and their extension into 3D nano-architectures [5]. Particular emphasis will be placed on giant nonreciprocity in superconductor-ferromagnet heterostructures, where magnetic flux quanta (Abrikosov vortices, or fluxons) interact with propagating spin excitations (spin waves, or magnons) in adjacent magnetically ordered media [6], allowing for their detection and generation [7].

[1] R. Feynman, The Feynman Lectures on Physics, 1 (1963) 46.
[2] F. Ando et al, Observation of superconducting diode effect, Nature 584 (2020) 373.
[3] B. Pal et al, Josephson diode effect from Cooper pair momentum, Nat. Phys. 18 (2022) 1228.
[4] F. Porrati et al, Vortex ratchet effect in a NbC strip with a periodic edge indentation, Small Methods e01430 (2025).
[5] I. Bogush et al, Vortex ratchet effect in superconductor open nanotubes and 3D nanoflakes, Rap. Res. Lett. 2500139 (2025).
[6] O. Dobrovolskiy et al, Magnon-fluxon interaction in a ferromagnet/superconductor heterostructure, Nat. Phys. 15 (2019) 477.
[7] O. Dobrovolskiy et al, Moving Abrikosov vortex lattices generate sub-40 nm magnons, Nat. Nanotechn. 20 (2025) 1764.

501	**Competition Between Singlet Formation and Nagaoka Ferromagnetism in a Quadruple Quantum Dot Array**	Emil Siuda	Contributed talk (16:30-16:45)

Emil Siuda (1) Ireneusz Weymann (1)

(1) Adam Mickiewicz University in Poznań

The interplay between superconductivity and magnetism remains one of the central problems of condensed matter physics, particularly in nanoscale systems where strong electron correlations play a dominant role. A prominent example of interaction-driven magnetism is Nagaoka ferromagnetism, which arises purely from electron correlations in nearly half-filled systems [1,2], and which has recently been experimentally realized in quantum dot plaquettes [3]. When such systems are coupled to a superconducting reservoir, the ferromagnetic state competes with singlet-forming pairing correlations, leading to nontrivial many-body behavior [4].
In this work, we investigate a quadruple quantum dot array proximitized by an s-wave superconductor and coupled to a normal metallic lead, providing a minimal platform to study the competition between Kondo correlations, superconducting pairing, and Nagaoka ferromagnetism. Focusing on the subgap regime, we determine the phase diagram of the system as a function of the coupling to the superconducting substrate and show that the proximity-induced pairing modifies the ferromagnetic ground state, leading to its suppression beyond a critical coupling strength. The presence of the normal lead introduces

an additional screening channel, resulting in a competition between Kondo correlations, superconductivity, and Nagaoka ferromagnetism, which gives rise to a new phase absent in isolated or weakly coupled systems. At the same time, high-spin states remain robust over a wide parameter range, indicating the persistence of Nagaoka-type ferromagnetism despite competing singlet correlations.
Our results demonstrate that hybrid quantum dot arrays provide a highly tunable platform for studying competing many-body phenomena and reveal how interaction-driven ferromagnetism evolves in the presence of superconducting correlations and coupling to external reservoirs.

[1] Nagaoka, Y. (1966). Ferromagnetism in a narrow, almost half-filled s band. Physical Review, 147(1), 392.
[2] Buterakos, D., & Sarma, S. D. (2019). Ferromagnetism in quantum dot plaquettes. Physical Review B, 100(22), 224421.
[3] Dehollain, J. P., Mukhopadhyay, U., Michal, V. P., Wang, Y., Wunsch, B., Reichl, C., ... & Vandersypen, L. M. (2020). Nagaoka ferromagnetism observed in a quantum dot plaquette. Nature, 579(7800), 528-533.
[4] Siuda, E., & Weymann, I. (2025). Competition between Nagaoka ferromagnetism and superconducting pairing in hybrid quantum dots. Sci. Rep., 15(25349), 25349.

575	**Complete delocalization in disordered Hatano-Nelson chains**	Sergej Flach	Invited talk (16:45-17:15)

Sergej Flach (1)

(1) Institute for Basic Science, Daejeon

The unidirectional Hatano-Nelson chain serves as the fundamental non-Hermitian building block of the Su-Schrieffer-Heeger (SSH) model. We investigate its Anderson localization properties under diagonal binary disorder. For weak disorder, the complex eigenvalue spectrum forms a single closed loop, which bifurcates into two distinct loops at a critical disorder threshold. Correspondingly, the spectral winding number undergoes a transition from 1 in the weak-disorder regime, through 1/2 at the critical point, to 0 in the strong-disorder limit. We show that the eigenstates are subexponentially localized, with a localization length that varies analytically as a function of the loop parameter. Notably, at weak and critical disorder, the spectrum hosts two completely delocalized states with diverging localization lengths. These findings remain robust under various boundary conditions, with the exception of strictly open boundaries. We also discuss to more complicated disorder, relate these findings to generalized Cassini ovals, and generalize to arbitrary lattice dimensions and Hermitian or non-Hermitian models with correlated hopping and onsite disorder.

161	**Hydrodynamics and entanglement under inhomogeneous driving**	Victor Eisler	Contributed talk (17:15-17:30)

Viktor Eisler (1) Riccarda Bonsignori (2) Stefano Scopa (3)

(1) University of Graz
(2) TU Graz
(3) LPENS

Time evolution and transport properties of integrable quantum many-body systems has been the topic of numerous investigations. While the hydrodynamic description starting from inhomogeneous initial states has been largely understood, much less is known about the setup where the time evolution operator itself is nonuniform. We present results for a chain of noninteracting fermions in two different setups: with periodically modulated hopping amplitudes, or a chemical potential gradient with arbitrary time-dependent slope. It is demonstrated that both cases admit a hydrodynamic description, while the driven ramp even allows for a complete analytic solution on the lattice. Moreover, we also show how these results help us to understand entanglement spreading along the chain.

211	**Quantum vs thermal fluctuations in phase transitions of two-dimensional superconductors**	Andrea Ponticelli	Contributed talk (17:30-17:45)

Andrea Ponticelli (1) Francesco Giuseppe Capone (1) Vittorio Cataudella (1) Antonio De Candia (1) Giulio De Filippis (1) Carmine Antonio Perroni (1)

(1) Università degli Studi di Napoli Federico II

We investigate the impact of quantum and thermal phase fluctuations on the suppression of superconducting order in two-dimensional systems. Within the two-dimensional quantum XY model in the phase representation, where on-site interaction terms govern quantum phase fluctuations, we perform extensive path-integral quantum Monte Carlo simulations. The resulting temperature–interaction phase diagram establishes the presence of a well-defined critical line ending at a quantum critical point at vanishing temperature with no indication of reentrant behavior. We further demonstrate that the resistance above the critical line reproduces the two expected different critical behaviors. For stronger interactions, above the quantum critical point, the system exhibits a crossover to an insulating regime at low temperatures. Finally, Monte Carlo calculations of current–current correlation functions enable us to extract the frequency-dependent conductivity in both superconducting and normal regimes, revealing a finite-frequency response that we attribute to quantum phase fluctuations.

M05 – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
347 **P042**	**Geometric Approach to Zero-Memory Quantum Dot Reservoir Computing**	Bongsu Kim	Poster

Bongsu Kim (1) Kun Woo Kim (1) Oscar Lee (2)

(1) Department of Physics, Chung-Ang University, 06974 Seoul, Republic of Korea
(2) London Centre for Nanotechnology, University College London, London WC1H 0AH, United Kingdom

Physical reservoir computing offers an energy-efficient alternative to conventional neural networks, where the intrinsic memory capacity within the physical system plays a central role. In this work, we demonstrate that memory capacity can be engineered extrinsically in memoryless systems by exploiting the

computational space-time tradeoff, substituting temporal memory with spatial degrees of freedom. Our approach utilizes multidimensional input nodes to function as a spatial memory axis, thereby removing the dependency on intrinsic history-dependent dynamics in the reservoir. We validate this framework through numerical simulations of a generalized single quantum dot, whose discrete energy states provide strong nonlinearity crucial for reservoir computing as well. To extract the processed information, we read out local observables equivalent to transport spectroscopy, accounting for the interaction between the system and measurement apparatus. By coupling this inherent nonlinearity with our extrinsic memory, we show that memoryless quantum reservoir can achieve high performance on both chaotic Mackey-Glass future prediction and nonlinear transformation tasks. Furthermore, by analyzing the geometry of the quantum state trajectories, we identify the physical mechanism underlying this memory emergence: extrinsic memory constructs a hysteresis loop within the quantum Hilbert space, and this loop becomes topologically stable when the evolution of the system state synchronizes with the input signal's frequency. Our work decouples reservoir computing from material-specific memory properties, significantly expanding the range of candidate systems for quantum neuromorphic computing.

460 **P043**	**Current precision in interacting hybrid Normal-Superconducting systems**	Nahual Sobrino	Poster

Nahual Sobrino (1) Rosario Fazio (2) Michele Governale (3) Fabio Taddei (4)

(1) International Centre For Theoretical Physics, Trieste
(2) Dipartimento di Fisica, Università di Napoli “Federico II”
(3) Victoria University of Wellington
(4) NEST, Istituto Nanoscienze-CNR and Scuola Normale Superiore, Pisa

We study Andreev-mediated transport and current fluctuations in interacting normal–superconducting quantum-dot systems. Using a generalized master equation based on real-time diagrammatics and full counting statistics, we compute the steady-state current, zero-frequency noise, and rate of entropy production in the large superconducting-gap limit. We show how Coulomb interactions modify Andreev-mediated transport by renormalizing resonant conditions and suppressing superconducting coherence, leading to a pronounced reduction of current precision even when average currents are only weakly affected. These effects are particularly evident at high temperatures, where conventional Coulomb-blockade features are thermally smeared while fluctuation properties remain highly sensitive. By analyzing thermodynamic uncertainty relations, we demonstrate that violations of the quantum bound present in the noninteracting regime are progressively reduced and eventually suppressed as interactions increase, whereas the recently proposed hybrid bound remains satisfied. Our results clarify how Coulomb interactions, and nonequilibrium fluctuations jointly determine transport properties in hybrid superconducting devices, and establish current precision as a robust benchmark for interacting Andreev transport beyond the noninteracting limit.

M06 - Interaction Effects in Correlated Systems with Higher-Order Van Hove Singularities and Flat Bands

M06 – Session 1 (Tue 22, 10:30-12:30, Chair: Joseph Betouras)			
ID	Title	Speaker	Type
674	**Signatures of heavy and light electrons in Magic Angle Twisted Bilayer Graphene**	E. Bascones	Invited talk (10:30-11:00)

E. Bascones (1) M.J. Calderón (1) A. Camjayi (2)

(1) Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)
(2) Universidad de Buenos Aires and Conycet

The topological character of the flat bands of twisted bilayer graphene (TBG) underlies the plethora of correlated phenomena found as a function of doping and temperature. Particularly, it determines the unconventional reorganization of the electronic spectrum, observed in the electronic cascades and detected with STM, inverse compressibility, transport and in the electronic bands recently measured with the Quantum Twisting Microscope (QTM). Our Dynamical Mean Field Theory + Hartree (DMFT+H) calculations on a heavy-fermion like model [1] with topologically fragile flat bands compare very well with STM, QTM, resistivity and inverse compressibility measurements [2,3]. At the heart of the strong electronic reorganization lies the formation of unconventional moments and heavy quasiparticles and a non-monotonic filling of the light electrons with increasing doping. After reviewing these properties and our predictions for the fingerprints in the optical spectrum and real space electronic properties that can be probed in future experiments, I will focus in our recent calculations at very low temperatures.

[1] M.J. Calderón and E. Bascones, PRB 102, 155149 (2020)
[2]A. Datta, M.J. Calderón, A. Camjayi and E. Bascones, Nat. Com 14, 5036 (2023)
[3] M.J. Calderón, A. Camjayi, A. Datta and E. Bascones, PRB-Letter 112, L041126 (2025)
[4] A. Camjayi, M.J. Calderón and E. Bascones, in preparation

670	**Charge and Spin order in the generalized Wigner crystal phase in twisted bilayer $MoTe_2$**	Arindam Pramanik	Contributed talk (11:00-11:15)

Arindam Pramanik (1) Andrzej Biborski (1) Michał Zegrodnik (1)

(1) AGH University of Krakow

Recent experiments in twisted bilayer MoTe2 (t-MoTe2) have uncovered many correlation-driven phases at various hole filling factors. The phases like fractional Chern Insulator, quantum anomalous Hall phase, superconducting states, and generalized Wigner crystal phase have been confirmed by multiple experimental studies. The majority of these phases are observed at either integer fillings or fractional fillings less than 1. However, one of the recent experimental findings shows correlated insulating states at fillings 4/3 and 3/2 for samples with 3.83o twist, which were interpreted as possible charge density wave states.
In our work, we have focused on revealing the exact nature of the insulating states at 4/3 and 3/2 fillings. We have studied the 2-band interacting model of the system to investigate the charge and spin order of these states. We employed unrestricted Hartree-Fock formalism in the real-space, allowing for spontaneous symmetry breaking without imposing any predefined supercell structure.
Our detailed analysis shows that the t-MoTe2 system possesses a very rich phase diagram in terms of general Wigner crystal phases as a function of twist angle and the strength of the applied displacement field. While the majority of the phase space is dominated by various $\sqrt{3}x\sqrt{3}$ ordered states, 2x2 ordered states appear when the displacement field is negligible. We found that the small and large twist systems are in the inter-valley coherent state (IVC) and valley polarized state (VP), respectively. The IVC to VP transition happens at 1.5o twist for both 4/3 and 3/2 fillings. The transition between any two ordered states can be tracked by the evolution of quantities like layer-polarization, spin-polarization, total energy, etc. Analysis of such quantities shows that all the transitions in our phase diagram are first-order in nature.

655	**Quantum criticality and emerging universality in flat band systems**	Qimiao Si	Invited talk (11:15-11:45)

Qimiao Si (1)

(1) Rice University

Quantum materials research is experiencing major advances in both depth and breadth [1]. Flat bands, in particular, emerge in a diverse range of materials, spanning twisted heterostructures and compounds with geometrically frustrated lattices. They feature strong correlation effect alongside non-trivial topology. Recent experiments on active-flat-band kagome and pyrochlore metals have uncovered non-Fermi liquid behavior [2], while the discovery of superconductivity in TMD moiré systems has likewise generated much excitement. Here, we theoretically investigate the correlation phenomena in d-electron-based metals on frustrated lattices [3], and discuss the similarities and differences with the physics of TMD moiré systems [4]. The shared methodology we have developed is in terms of the notion of compact molecular orbitals, which enable effective models in the form of topological Kondo lattice models [3,4]. Accordingly, we advance the understanding of strange metallicity and unconventional superconductivity, while also suggesting a broader principle that topology induces quantum fluctuations and thus leads to new correlation physics. Together with the complementary advancements on Weyl-Kondo semimetals [5], these studies point toward a broader perspective that strong correlations and topology form a two-way road towards new states of quantum matter.

[1] S. Paschen & Q. Si, Nat. Rev. Phys. 3, 9 (2021); H. Hu et al., Nat. Phys. 20, 1863 (2024).
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[5] H.-H. Lai et al., PNAS 115, 93 (2018); H. Hu et al., arXiv:2110.06182; D. M. Kirschbaum, L. Chen et al., Nat. Phys. 22, 218 (2026)

100	**Triplet superconductivity supported by an X9 high-order Van Hove singularity**	Chethan Sanjeevappa	Contributed talk (11:45-12:00)

Chethan Sanjeevappa (1) Joseph J. Betouras (1) Anirudh Chandrasekaran (1,2)

(1) Department of Physics, Loughborough University
(2) Max Planck Institute for Solid State Research, Stuttgart

High-order Van Hove singularities significantly enhance correlation effects due to their strongly divergent density of states, thereby providing natural platforms for interaction driven instabilities. In this work, we focus on a single fourfold-symmetric high-order Van Hove singularity of X_9 type situated close to the Fermi surface. We analyse the possibility of a superconducting state in the presence of nominally weak Hubbard interactions, via the Kohn-Luttinger type mechanism. We find that the leading instability occurs in the triplet p-wave channel with critical temperature scaling as T_c ∝ U^2. We discuss the fluctuations in connection to lower dimensionality, and the condition to stabilise a triplet superconducting state. Our results are relevant to the benchmark quantum material Sr_3Ru_2O_7 which hosts an X9 singularity in the presence of an external magnetic field, and we estimate an upper bound on the critical temperature in this system. More broadly, our work suggests a potential route to superconductivity in materials capable of hosting an X_9 singularity.

Work to appear in Physical Review Research, DOI: https://doi.org/10.1103/jdr9-4f95
The work has been supported by the UK Engineering Physical Sciences Research Council grants EP/T034351/1 and EP/X012557/1.

664	**Bilayer Kagome with Incommensurate Twisting: The Emergence of Higher-Order Magic Angles**	David Perkins	Contributed talk (12:00-12:15)

David Perkins (1) Joseph J. Betouras (1)

(1) Department of Physics, Loughborough University

Twisting in van der Waals heterostructures has proven itself as indispensable in engineering new technologies with bespoke properties, from the tuning of proximity effects and spin transport to the enabling of superconductivity and non-trivial topology [1-4]. Twisted bilayer graphene has been the forerunner in our exploration of twistronics, but twisting in non-honeycomb systems has now become a new focal point in the field [5,6]. Most recently, twisted bilayer kagome (TBK) has emerged as a new point of interest due to the appearance of kagome patterning and physics in metal-organic frameworks and rare-Earth compounds [7,8]. The study of small incommensurate twists from a continuum perspective has relied heavily on the Bistritzer-MacDonald (BM) formalism to construct a moiré Hamiltonian. This method requires a non-extended Fermi surface, making application to TBK more challenging due to the kagome monolayer's flat band.
In this talk, we extend the BM model to arbitrary twisted bilayer systems and apply it to TBK near 1/3 filling. We demonstrate an approximate particle-hole symmetry in TBK and show that TBK possesses higher-order magic angles corresponding to the onset of higher-order Van Hove singularities, evidenced by a drastic reduction in the renormalised Fermi velocity. We further discuss the topology of the emergent moiré bands and the role of sublattice interference at finite temperature.

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[2] D.T.S. Perkins et al., Phys. Rev. B 109, L241404 (2024).
[3] Y. Cao et al., Nature 556, 43 (2018).
[4] Z. Song et al., Phys. Rev. Lett. 123, 036401 (2019).
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[6] D.T.S. Perkins et al., Phys. Rev. B 112, 235134 (2025).
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M06 – Session 2 (Wed 23, 10:30-12:30, Chair: Silke Buehler-Paschen)

ID	Title	Speaker	Type
203	**Observation of Anomalous Thermal Hall Effect in a Kagome Superconductor CsV_3Sb_5**	Minoru Yamashita	Invited talk (10:30-11:00)

Minoru Yamashita (1)

(1) ISSP, University of Tokyo

Spontaneous time-reversal symmetry (TRS) breaking is one of the interesting cooperative phenomena brought by a phase transition in solids, which allows both a spontaneous magnetic moment as observed in a ferromagnet and a chiral edge flow to be realized. Of particular interest in the chiral flow by the broken TRS is the topologically-protected edge current in a chiral superconductor in which spontaneous magnetic moment appears by forming Cooper pairs with a finite orbital angular momentum. In contrast, conventional superconductivity is incompatible with collective magnetism and broken TRS. Although a charge current is not conserved in a superconductor, a thermal current brought by Bogoliubov quasiparticles is conserved, giving rise to a quantization of the thermal Hall conductivity in a chiral superconductor by the Chern number characterizing the chiral superconducting state. In addition to such an intrinsic anomalous thermal Hall effect (ATHE), extrinsic ATHEs by impurity scatterings are also suggested in chiral superconductors. Although numerous candidate materials have been reported so far to realize chiral superconductivity, mainly by the observation of the spontaneous magnetization by the polar Kerr or the μSR measurements, these ATHEs have yet to be observed.
In this presentation, I will report our successful observation of an ATHE developing below the superconducting transition temperature at zero external magnetic field in the kagome-lattice superconductor CsV_3Sb_5 [1]. The anomalous thermal Hall conductivity (κ_{xy}^{ATHE}) is determined by measuring the transverse temperature difference caused by a thermal current at zero external field, after cooling the sample under a finite magnetic field at the superconducting transition to polarize the domains of the chiral superconductor. Reversing this "training" field allows us to estimate κ_{xy}^{ATHE} by

antisymmetrizing the transverse thermal-Hall resistance to remove the mixed longitudinal component. We verify our experimental setup by confirming the null result for the conventional type-II superconductor 2H–NbS_2. We further exclude the effects of trapped fluxes in the sample by measuring the training-field dependence of the trapped field by micro-Hall array measurements. Our results demonstrate that the magnitude of κ_{xy}^{ATHE} observed in CsV3Sb5 exceeds the theoretical value expected for an intrinsic ATHE of a chiral superconductor by more than one order of magnitude, as well as exhibits a different temperature dependence of κ_{xy}^{ATHE} from that of an intrinsic ATHE. On the other hand, both the magnitude and the temperature dependence of κ_{xy}^{ATHE} are consistent with an extrinsic impurity-induced ATHE that predicts a temperature dependence of κ_{xy}^{ATHE} with a peak at a fraction of the superconducting transition temperature without the residual of κ_{xy}^{ATHE}/T depending on the impurities, suggesting observation of extrinsic ATHE in a chiral superconducting state in CsV_3Sb_5. The method we use to observe the ATHE is applicable to various superconductors, which will bring substantial advances in the research on chiral superconductivity.

[1] H. Yoshida et al., Sci. Adv. 11, eadu2973 (2025)

650	**A hierarchy of interactions – effect of lattice, orbital and band geometry on electronic interaction in Kagome superconductors**	Anirudh Chandrasekaran	Contributed talk (11:00-11:15)

Anirudh Chandrasekaran (1) Laura Classen (1)

(1) Max Planck Institute for Solid State Research

We derive a set of general formulae for projecting a real space electronic interaction $V(\boldsymbol{r})$ on to orbital resolved bands in 3D, layered and monolayer lattices. The resulting k-space interaction $V(\boldsymbol{k}_1, \boldsymbol{k}_2, \boldsymbol{q}, n_1, n_2, n_3, n_4)$ resembles a vertex function, with momentum conservation up to a reciprocal lattice vector and an explicit dependence on the bands n_1, n_2, n_3 and n_4 corresponding to the ingoing and outgoing electrons. We apply this formalism to tight-binding models with higher order van Hove singularities, that are relevant to materials like the Kagome superconductors. We show that a general feature of such a band-projected interaction is that some k-space scatterings $\boldsymbol{k}_1, \boldsymbol{k}_2 \rightarrow \boldsymbol{k}_1 + \boldsymbol{q}, \boldsymbol{k}_2 - \boldsymbol{q}$ are accompanied by a much stronger interaction as compared to others. Such a hierarchy of interactions essentially results from the modulation of the real space interaction by lattice, orbital and band geometries. This can facilitate a more nuanced correlated-electron calculation with mean-field, parquet and functional renormalization group methods.

657	**ARPES Investigation of Electronic Structure in MT_6X_6 Kagome Compounds**	Chan-young Lim	Contributed talk (11:15-11:30)

Santiago Blanco-Canosa (1) Chan-young Lim (1) Ji Dai (2) Subarna Das (3) Jonathan D. Denlinger (4) Claudia Felser (3) Artem Korshunov (1) Avdhesh Kumar Sharma (3) Chandra Shekhar (3) Massimo Tallarida (2)

(1) Donostia International Physics Center
(2) ALBA Synchrotron Light Source
(3) Max-Planck-Institute for Chemical Physics of Solids
(4) Advanced Light Source

Kagome lattice systems host Dirac dispersions, flat bands, and van Hove singularities near the Fermi level, making them a model setting for correlated electronic behavior. Here, we present an angle-resolved photoemission spectroscopy (ARPES) study of kagome 166 compounds, including LuFe6Ge6, LuCr6Ge6, HoCr6Ge6, and ScNi6Ge6, most of which have not been previously investigated by ARPES. We resolve kagome-derived electronic states characterized by Dirac-like dispersions, flat band features, and saddle points in close proximity to the Fermi energy. While these materials share a common band structure framework, systematic variations in band filling and exchange splitting lead to distinct Fermi-surface topologies and tunable proximity to van Hove singularities. These results highlight kagome 166 systems as a platform for investigating the interplay between lattice geometry, magnetism, and electronic instabilities.

791	**Kekulé order from diffuse nesting near higher-order Van Hove points**	Ronny Thomale	Invited talk (11:30-12:00)

Ronny Thomale (1)

(1) Theoretische Physik I, Julius-Maximilians-Universität Würzburg

Translation symmetry-breaking order is assumed to be suppressed by the lack of Fermi surface nesting near certain higher-order Van Hove singularities (HOVHS). We show the anisotropic band-flattening inherent to such HOVHS, combined with broadening of the Fermi surface due to elevated critical temperatures, results in the Fermi surface becoming approximately nested at a wavevector unrelated to the precise shape of the Fermi surface - leading to a Kekulé density wave formation. The effect is demonstrated using unbiased renormalization group calculations for a model of the breathing kagome lattice. Our mechanism - termed diffuse nesting - represents an entirely new notion in the study of Fermi surface instabilities.

706	**Superconductivity in kagome metals from loop current fluctuations**	Daniel Schultz	Contributed talk (12:00-12:15)

Rafael Fernandes (1) Yong Baek Kim (2) Asimpunya Mitra (2) Grgur Palle (1) Jörg Schmalian (3) Daniel Schultz (3)

(1) University of Illinois Urbana-Champaign
(2) University of Toronto
(3) Karlsruhe Institute of Technology

We demonstrate that soft fluctuations of translation symmetry-breaking loop currents provide a mechanism for unconventional superconductivity in kagome metals that naturally addresses the multiple superconducting phases observed under pressure. Focusing on the rich multi-orbital character of these systems, we show that loop currents involving both vanadium and antimony orbitals generate low-energy collective modes that couple efficiently to electrons near the Fermi surface and mediate attractive interactions in two distinct unconventional pairing channels. While loop-current fluctuations confined to vanadium orbitals favor chiral d+id superconductivity, which spontaneously breaks time-reversal symmetry, the inclusion of antimony orbitals stabilizes an s± state that is robust against disorder. We argue that these two states are realized experimentally as pressure increases and the antimony-dominated Fermi surface sheet undergoes a Lifshitz transition.

687	**The magnetotropic response of the kagome metal CsV_3Sb_5 in its superconducting and metallic states**	Mohammad Sameer	Contributed talk (12:15-12:30)

Shiva Safari (1) Kimberly Modic (1) Mohammad Sameer (1)

(1) Institute of Science and Technology, Austria

The kagome superconductor CsV_3Sb_5 ($T_c \approx 2.5$ K) hosts a 2×2×2 charge density wave below 94 K[1] and signatures of electronic nematicity and time-reversal-symmetry breaking near 30 K. The interplay of these orders with its superconducting state and Fermi-surface topology remains an open question.
Using resonant torsion magnetometry, we investigate CsV_3Sb_5 single crystals between 0.7–35 K and 0–14 T. The technique measures the angular curvature of the free energy $k = \partial^2 F/\partial\theta^2$ via resonant-frequency shifts $\Delta f(B, T, \theta)$.
Angular sweeps from out-of-plane to in-plane orientations resolve clear de Haas–van Alphen oscillations superimposed on the uniaxial magnetotropic background. Field sweeps below T_c reveal a pronounced peak inside the superconducting state. The field positions of this peak define a phase boundary $H_1(T)$ internal to the superconducting region, distinct from published $H_{c2}(T)$ curves. At fields above H_{c2}, the magnetotropic amplitude exhibits a curvature change near $T \approx 25$ K of yet-unestablished origin.
In-plane angular measurements are currently underway to clarify if nematicity is an intrinsic, bulk property of CsV_3Sb_5, or if there are any additional symmetries broken below 35 K.
In-plane angular measurements at fixed polar angle are currently underway to clarify the microscopic origin of rotational symmetry breaking in this material.

[1] Z. Liang et al., Phys. Rev. X 11, 031026 (2021).

M06 – Session 3 (Thu 24, 10:30-12:30, Chair: Peter Wahl)

ID	Title	Speaker	Type
676	**Modifying low-energy electronic states to control superconductivity in artificial two-dimensional systems**	Tetsuo Hanaguri	Invited talk (10:30-11:00)

Tetsuo Hanaguri (1) Tadashi Machida (1) Masahiro Naritsuka (1)

(1) RIKEN CEMS

Superconducting properties can be controlled by various external parameters, such as doping and pressure, which modify low-energy electronic states. In particular, materials hosting singularities in the density of states near the Fermi level are expected to be susceptible to small changes in external parameters. Here, we employ ultralow-temperature scanning tunneling microscopy and spectroscopy to investigate artificial two-dimensional systems that offer unique routes for controlling superconductivity. In the Rashba surface superconductor Si(111)-$\sqrt{3} \times \sqrt{3}$-(Tl, Pb), both conventional and unconventional pairing states have been proposed. High-resolution quasiparticle interference imaging reveals a van Hove singularity (VHS) in close proximity to the Fermi level. We speculate that this VHS plays a crucial role in the pairing interaction, which can be modified by slight shifts of the Fermi level relative to the VHS through doping of the Si(111) substrate [1].
We also investigate monolayer $NbSe_2$ on graphene, where the superconducting gap can be controlled by the twist angle, which determines the degree of Fermi surface overlap between $NbSe_2$ and graphene [2]. By developing an in-situ twist-angle tuning technique, we reveal the detailed angular dependence of the superconducting gap.

[1] T. Machida, et al., Phys. Rev. B 105, 064507 (2022).
[2] M. Naritsuka et al., Nature Phys. 21, 746-753 (2025).

777	**Scanning Tunneling Microscopy in high vectorial magnetic fields**	Jaime Rumeu Ozores	Contributed talk (11:00-11:15)

Jaime Rumeu Ozores (1)

(1) Laboratorio de Bajas Temperaturas y Altos Campos Magnéticos, Departamento de Física de la Materia Condensada, Instituto Nicolás Cabrera and Condensed Matter Physics Center (IFIMAC), Unidad Asociada UAM-CSIC, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

Cryogenic Scanning Tunneling Microscopy (STM) has been instrumental in the development of scanning probe microscopies. The addition of a magnetic field opens new prospects, such as the observation of vortex lattices in superconductors or of Landau quantization. For the latter, it is of particular importance to decrease as far as possible the size of the STM. Although efforts made during past years have led to some improvements, the size is still far above the typical sizes available for instruments used in high magnetic fields. Here we discuss the development of both a reduced size STM and a rotating platform meant to obtain measurements at different angles between the sample and the magnetic field[1]. This feature will allow us to observe new exotic phases emerging at high tilted magnetic fields, unreachable using state of the art three-axis coils [2]. Both the head and the base of the main body of the STM have been manufactured through 3D printing in grade 3 Titanium, which could turn out to be a good method to optimize the weight without modifying too much the stiffness of the microscope. Finite element calculations of the 3D printed system support the latter aspect. The STM has a diameter of 16 mm and a height of 25 mm. We have successfully tested the stability of the system by reproducing millions of atomic-sized gold junctions at fields of 8 T in different orientations. We have also obtained images of the tilted vortex lattice and achieved atomic resolution in 2H-NbSe2, demonstrating the proper functioning of the rotatory system together with the STM. Having set-up this ultra-small size STM will also allow its use in high magnetic field facilities. Further improvements, as the construction in shapal or ceramics to avoid Joule heating, are on the way.

[1] J. Rumeu Ozores, et al.Rev. Sci. Instrum. 97, 033705 (2026).
[2] F. Martín Vega, et al. Rev. Sci. Instrum. 92, 103705 (2021).

788	**A data-driven approach to correlated two-dimensional materials**	Agnes Valenti	Invited talk (11:15-11:45)

Agnes Valenti (1)

(1) Flatiron Institute, Center for Computat Quantum Physics, New York, NY 10010 USA

Two-dimension van-der-Waals materials provide a versatile platform with a high degree of tunability, that has led to a multitude of realizations of correlated and topological phases in the recent years. However, theoretical modeling remains a challenge: Strong correlations call for tools beyond mean-field theory. In this talk I will explain how variational Monte Carlo, in particular neural quantum states, addresses this challenge. I will use these tools to piece together features such as anisotropy or quantum geometry in 2D quantum materials and explain their effect on the emerging phases. I will then explain how modern machine learning advances can be used to shape new tools for the exploration of strongly correlated materials.

683	**Signatures of coupling to bosonic modes in quasiparticle interference**	Carolina de Almeida Marques	Contributed talk (11:45-12:00)

Carolina de Almeida Marques (1)

(1) School of Physics and Astronomy, University of St Andrews

Interaction effects in strongly correlated electron materials stabilize emergent electronic phases that promise the next technological revolution, such as superconductivity, Mott insulating states and density wave orders. To gain insight into the origin of these states and learn how to manipulate them, a deep understanding of their electronic structure and coupling to lattice and spin degrees of freedom is needed. However, the presence of the same interactions that lead to this rich physics hinders a simple identification of the underlying band structure, as they lead to broadening and additional features in spectroscopic techniques such as angle resolved photoemission spectroscopy (ARPES) and scanning tunnelling microscopy (STM).
Electronic interaction effects are encoded in the self-energy which can incorporate the effects of different types of interactions, such as Coulomb repulsion U, electron-phonon coupling and Hund's coupling J. While the self-energy results in broadening and renormalization of the electronic dispersion, the inelastic processes result in replica features related to the energy of bosonic modes.
I will discuss the effects of electron-boson coupling and self-energy in correlated materials, and show how the latter can be accounted for by introducing them in calculations of quasiparticle interference as measured by STM. I will show how the self-energy and inelastic effects affect the scattering patterns, how to extract information from them and infer on the type of interactions that dominate the tunneling process and electronic interactions in the sample.

787	**Valley-Selective Correlated Insulator in twisted double bilayer WSe_2**	Abhay Pasupathy	Invited talk (12:00-12:30)

Abhay Pasupathy (1)

(1) Columbia University

A number of moiré bilayer semiconductors display insulating phases at a filling of one carrier per unit cell ("half-filling"). We understand these insulating states to be driven by strong electronic correlations. It is generally understood that electron screening reduces these correlations, and so these states have been seen in isolated flat band systems. In this work, I will describe recent experiments on twisted double bilayer WSe, which is an interesting moiré semiconductor that has two separate hole valleys near the zone center and zone boundary. The energy separation between the tops of these valleys can be sensitively controlled using an out of plane electric field. It is thus possible to realize situations where one of the valleys is half-filled, while the other valley has some arbitrary filling. We show that it is possible to have an insulating state formed in one valley while the other continues to remain itinerant - ie, to realize a valley-selective correlated insulator.

M07 - Nickelate Superconductors: A New Platform for Unconventional Cooper-Pairing

M07 – Session 1 (Mon 21, 16:00-18:00, Chair: Ilya Eremin)			
ID	Title	Speaker	Type
563	**High-field reentrant and hysteretic superconducting states in an infinite-layer nickelate**	A. Ariando	Invited talk (16:00-16:30)

Ariando Ariando (1)

(1) National University of Singapore

Magnetism is generally detrimental to superconductivity, but in unconventional systems the two coexist and give rise to exotic phenomena such as spin-triplet pairing and field-induced superconductivity. In the infinite-layer nickelate series $SmEuCaNiO_2$ (SECNO), samples with specific Eu concentrations exhibit field-reentrant superconductivity, which has been attributed to Jaccarino-Peter (JP) compensation driven by Eu^{2+} magnetic moments.
In this talk, I will further present a striking observation of a hysteretic superconducting state in SECNO, emerging below 2 K with coercive field exceeding 1 T, unprecedented among known ferromagnetic superconductors or superconducting heterostructures. Complementary evidence, together with the Eu-concentration dependence, points to an intrinsic underlying ferromagnetic ground state spanning the SECNO series. By revealing the coexistence of ferromagnetism and superconductivity, our work provides critical insights into the interplay among ferromagnetic order, JP compensation, and Eu doping in SECNO. This field-history-dependent superconducting state enriches the fundamental physics of correlated oxides.

389	**Rare-earth and electron doping in infinite-layer and perovskite nickelate thin films**	Marta Gibert	Invited talk (16:30-17:00)

Marta Gibert (1)

(1) TU Wien

The discovery of superconductivity in doped infinite-layer nickelate thin films has stimulated considerable interest in understanding the role of different dopants. Among these, magnetic rare-earth doping occupies a particularly distinctive position. Eu-doped $NdNiO_2$ gives rise to a striking field-induced re-entrant superconductivity, which emerges from a delicate balance between the competing spin polarizations of the Eu^{2+} and Nd^{3+} ions [1]. This interplay produces a net suppression of the internal magnetic field over an intermediate field range. To directly probe the underlying spin polarization of both magnetic species, X-ray magnetic circular dichroism (XMCD) measurements are employed.
Turning to the doping landscape more broadly, a notable asymmetry is apparent: existing studies of the 113-perovskite parent compound thin films have mainly concentrated on the hole-doped regime, with electron-doping investigations largely confined to bulk materials. To tackle this imbalance, a systematic study of electron doping in $NdNiO_3$ thin films via A-site substitution is presented. Pb is employed as a dopant, exploiting its valence-skipping character to inject electrons into the nickelate framework [2]. This work establishes A-site Pb substitution as a viable and controlled route to electron doping in rare-earth nickelate thin films.

[1] L. Varbaro et al. arXiv:2601.19473 (2026).
[2] M. Hadjimichael et al. Adv. Electron. Mater. 2201182 (2023).

671	**Electronic evolution throughout the topotactic reduction of nickelates: Insights from x-ray absorption spectroscopy**	Rebecca Pons	Contributed talk (17:00-17:15)

Rebecca Pons (1)

(1) Max Planck Institute for Solid State Research

The discovery of superconductivity in infinite-layer nickelates without alkaline-earth doping, as well as in Ruddlesden-Popper nickelates, raises the question of whether these cases are related and whether they are based on a common mechanism. For the infinite-layer nickelates a critical step is the topotactic reduction. We investigate the electronic configurations arising in the reduction process by employing soft x-ray absorption spectroscopy (XAS) on $PrNiO_x$ thin films with x=2-3 at various stages of topotactic reduction. A comparison of the Ni-L edge spectra, calculated using single and double cluster ligand-field models, shows that none of the measured samples can be described by the expected pure d^9 configuration. Even in the most reduced samples, the concomitant changes at the O-K edge upon reduction exhibit signs of remaining 2p holes. To quantify these findings, we analysed the Ni-L edge spectra using the charge sum rule and found that, in the maximally reduced films, the average number of 3d holes remained at 1.35. The superconducting samples have even higher average hole numbers, which calls into question hole doping levels assumed for cation doped infinite-layer nickelates and their similarity to the undoped superconducting compounds. Overall, XAS signatures for different reduction stages and configurations will be presented and different possible sources of the hole doping discussed.

90	**The RPA+DMFT approach for unconventional superconductivity: application to nickelate superconductors**	Hanghui Chen	Contributed talk (17:15-17:30)

Hanghui Chen (1,2)

(1) NYU Shanghai
(2) New York University

Spin fluctuations are widely believed to mediate electron pairing in unconventional superconductors. In gap-equation calculations, the random phase approximation (RPA) has been extensively used to construct the spin-fluctuation pairing potential that arises from Hubbard-like interactions. However, RPA is formally valid only in the weak-coupling regime and tends to predict spin-density-wave (SDW) instabilities at unrealistically small interaction strengths.

In this work, we extend RPA to intermediate and strong coupling by combining it with dynamical mean-field theory (DMFT), forming an approach we term RPA+DMFT. Within this framework, the bare susceptibility in RPA is replaced by a "dressed" susceptibility that incorporates quasiparticle dispersion and spectral weight obtained from DMFT. This dressed susceptibility is then used to construct the pairing interaction for the gap equation.
We apply the RPA+DMFT method to infinite-layer nickelates and find that the leading superconducting eigenvalue exhibits a non-monotonic dependence on interaction strength, peaking at intermediate coupling, in qualitative agreement with previous studies. Furthermore, we find that the orbital hybridization in infinite-layer nickelates leads to van Hove singularities (VHS) that are pinned to the Fermi surface. Those VHS brings the system closer to magnetic instability, amplifying antiferromagnetic spin fluctuations. This naturally explains why infinite-layer nickelates such as La0.8Sr0.2NiO2 exhibits a sizable superconducting transition temperature, despite the fact that the "self-doping" effect makes its Ni-dx2−y2 orbital overdoped relative to the phase diagram of cuprates.

Chengliang Xia, Shengjie Zhou, Hanghui Chen, "Three-dimensional fermi surface, van hove singularity and enhancement of superconductivity in infinite-layer nickelates", arXiv:2504.18778.

160	**ARPES spectra and the role of interstitial-s orbital in infinite-layer nickelates calculated by DFT+DMFT**	Leonard Verhoff	Contributed talk (17:30-17:45)

Karsten Held (1) Liang Si (1) Leonard Verhoff (1)

(1) TU Wien

Infinite-layer nickelates, such as $NdNiO_2$, are a compelling platform to explore the microscopic origin of unconventional high-temperature superconductivity, from both theoretical and experimental perspectives.
Experimentally, infinite-layer nickelates are reduced from the stable perovskite phase, leaving an empty apical oxygen site. Density functional theory (DFT) calculations show that the resulting interstitial vacancy hosts localized, *s*-like states about 2 eV above the fermi level, while recent angle-resolved photoemission spectroscopy (ARPES) measurements of superconducting $NdNiO_2$ thin films conjectured Fermi surfaces with major -like orbital character, highlighting a possible role of interstitial-*s* states in superconductivity.
We present DFT and dynamical mean field theory calculations of Fermi surfaces, directly comparable to ARPES spectra. Our ARPES simulations explicitly include first-principles photoemission matrix elements, capturing the impact of orbital shapes on the measured intensity. We show how the correlated band structure reproduces low-energy ARPES spectra and identify the features dominated by interstitial-*s* character.

We acknowledge support through a joint German and Austrian Science Funds (DFG and FWF) project; FWF project ID I5398.

273	**Stabilizing Magnetism in $NdNiO_2$ via Self-Doping**	Roman Drachynskyi	Contributed talk (17:45-18:00)

Wojciech Brzezicki (1) Roman Drachynskyi (1) Krzysztof Wohlfeld (2)

(1) Jagiellonian University
(2) University of Warsaw

We investigate magnetism in the electron-doped infinite-layer nickelate $NdNiO_2$ within a multi-orbital tight-binding framework including both Ni and Nd states. The model captures the self-doping effect arising from charge transfer into Nd bands. For realistic parameters, we find that undoped $NdNiO_2$ lies just outside the antiferromagnetic (AFM) region of the phase diagram, consistent with the absence of long-range order and the presence of short-range AFM correlations and broad magnetic excitations observed experimentally.
Electron doping markedly enhances the stability of AFM order via the self-doping mechanism, in clear contrast to the behavior of cuprates. For reduced charge-transfer energies, self-doping becomes stronger and stabilizes stripe-like configurations already at the mean-field level [1]. These results highlight the central role of Nd-derived states and suggest that incorporating correlation effects beyond conventional mean-field theory, for instance using so-called ghost-Gutzwiller approach [2], may provide a more complete quantitative description.

[1] Adam Kłosiński, Roman Drachynskyi, Krzysztof Wohlfeld, and Wojciech Brzezicki, Phys. Rev. B 113, 085148 (2026).
[2] Carlos Mejuto-Zaera and Michele Fabrizio, Phys. Rev. B 107, 235150 (2023).

We acknowledge support from the National Science Centre (NCN, Poland) under Projects No. 2021/43/B/ST3/02166 and No. 2024/55/B/ST3/03144.

M07 – Session 2 (Tue22, 16:00-18:00, Chair: Karsten Held)

ID	Title	Speaker	Type
51	**High-temperature superconductivity in pressurized Ruddlesden-Popper nickelates**	Meng Wang	Invited talk (16:00-16:30)

Meng Wang (1)

(1) Sun Yat-Sen University

The recent discovery of high-temperature superconductivity at 80 K in $La_3Ni_2O_7$ under high pressure has established nickelates as a new family of high-Tc superconductors, alongside the cuprates and iron-based systems[1-4]. This breakthrough has since been extended to other Ruddlesden-Popper nickelates under pressure and in thin-film form at ambient pressure. Our research group, working in collaboration with researchers worldwide, has been at the forefront of investigating the fundamental properties of these materials. Our studies, spanning both ambient and high-pressure conditions, have revealed a complex landscape featuring density-wave-like orders[4], structural transitions[5,6], strange metal behavior[1], and orbital-dependent electronic correlations[7,8]. Furthermore, we have explored the critical roles of oxygen vacancies[9], magnetic excitations[10], and doping in shaping the phase diagram. In this talk, I will review these key experimental discoveries and discuss the essential parameters that govern the emergence of high-Tc superconductivity in Ruddlenden-Popper nickelates, providing crucial insights into the mechanism of unconventional superconductivity.

[1] H. L. Sun, M. W. Huo et al., Nature 621, 493(2023)

[2] Y. N. Zhang, D. J. Su, Y. E. Huang et al., Nature Physics, 20, 1269(2024)
[3] J. Hou, P. T. Yang, Z. Y. Liu et al., Chinese Physics Letters 40, 117302(2023)
[4] Z. Liu, H. L. Sun, M. W. Huo, et al., Sci. China-Phys. Mech. Astron. 66, 217411(2023)
[5] L. H. Wang, Y. Li, S. Y. Xie et al., JACS 146, 7506(2024)
[6] J. Y. Li, D. Peng, P. Y. Ma et al., National Science Review, nwaf220 (2025)
[7] J. Yang, L. Zhao, M. Wang, X. J. Zhou et al., Nat. Commnu. 15, 4373(2024)
[8] Z. Liu, M. W. Huo, J. Li et al., Nat. Commnu. 15, 7570(2024)
[9] Z. H. Dong, M. W. Huo, J. Li et al., Nature 630, 847 (2024)
[10] T. Xie, M. W. Huo, X. S. Ni et al., Sci. Bull. 69, 3221(2024)

174	**Spectroscopic insights into the multiorbital character of density waves in Ruddlesden-Popper nickelate superconductors**	Mathias Hepting	Invited talk (16:30-17:00)

Matthias Hepting (1)

(1) Max Planck Institute for Solid State Research

Ruddlesden-Popper (RP) nickelates exhibit high-temperature superconductivity closely intertwined with charge and spin density-wave order. However, fundamental questions remain regarding the orbital character, symmetry, and gap formation associated with these density-wave instabilities. Using polarization-resolved Raman scattering on the trilayer compound $La_4Ni_3O_{10}$, we resolve characteristic phonon anomalies and a redistribution of electronic spectral weight across the density-wave transitions. Momentum-selective electronic Raman responses, combined with multiorbital model calculations, reveal a density-wave-induced gap with incoherent, non-mean-field-like opening and involvement from both Ni $d_{x^2-y^2}$ and d_{z^2} states [1]. These results help reconcile conflicting experimental reports on the density-wave gap and underscore its multiorbital character. In addition, I will discuss complementary Raman investigations of the monolayer-trilayer polymorph $La_3Ni_2O_7$, providing a broader perspective on how structural complexity within the RP series influences lattice dynamics and intertwined electronic instabilities [2].

[1] A. Suthar et al., arXiv:2508.06440
[2] V. Sundaramurthy et al., arXiv:2512.17583v1

307	**Advances in phase characterization and high-pressure susceptibility measurements of Ruddlesden-Popper nickelates**	Abhi Jigneshkumar Suthar	Contributed talk (17:00-17:15)

Abhi Jigneshkumar Sutha (1) Vignesh Sundaramurthy (1) Pascal Reiss (1) Pascal Puphal (1) Pablo Sosa-Lizama (1) Masahiko Isobe (1) Peter A. van Aken (1) Y. Eren Suyolcu (1) Hidenori Takagi (1) Bernhard Keimer (1) Matthias Hepting (1)

(1) Max Planck Institute for Solid State Research

Ruddlesden-Popper (RP) nickelates have recently attracted significant attention following the emergence of superconductivity under pressure. However, their interpretation is often complicated by phase intergrowth and oxygen non-stoichiometry in crystals grown by the optical floating-zone method. Reliable identification of the structural phase is therefore essential prior to spectroscopic, transport, or thermodynamic investigations. Here, we show that polarization-resolved Raman spectroscopy provides a rapid and sensitive probe for phase identification in RP nickelates. By systematically characterizing monolayer, bilayer, monolayer–trilayer polymorph, and trilayer compounds, we establish distinct spectral fingerprints that enable unambiguous discrimination between different RP members and their polymorphs, while also allowing assessment of sample quality in the presence of mixed phases.
In addition, we present the development of a high-pressure AC susceptibility setup employing a gasket-integrated coil design to probe the Meissner response of micron-scale samples inside a diamond anvil cell. Detecting superconductivity in nickelates is particularly challenging because of the small sample volume and the reported low superconducting volume fractions, in some cases below 1%, requiring substantial improvements in signal-to-noise ratio. The setup enables reproducible measurements without repeated coil fabrication or rewiring, thereby significantly reducing experimental overhead.
These developments establish a practical route toward reliable phase identification and quantitative probing of superconductivity in nickelates, providing a versatile platform for studying correlated materials under extreme conditions.

312	**Decoding Superconductivity in $La_3Ni_2O_{7-\delta}$ Thin Films via Ozone-Driven Structure and Oxidation Tuning**	Mathieu Flavenot	Contributed talk (17:15-17:30)

Mathieu Flavenot (1) Daniele Preziosi (1) Alexandre Gloter (2) Hoshang Sahib (3) Nathalie Viart (1) Laurent Schlur (1) Gilles Versini (1) Marc Lenertz (IPCMS) Jérôme Robert (1)

(1) Institut de physique et chimie des Matériaux de Strasbourg
(2) LPS, Universite Paris-Saclay
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The recent discovery of superconductivity below 80 K in bulk Ruddlesden–Popper (RP) $La_3Ni_2O_7$ (LNO327) under high pressure (>14 GPa) has reignited intense interest in nickel-based superconductors1. This breakthrough marks a new chapter in the “Nickel Age”, demonstrating superconductivity in a compound with a nominal $Ni^{2.5+}$ valence state and a non–square-planar coordination geometry, clearly distinct from both cuprates and infinite-layer nickelates (which are closer to $3d^9$). As such, LNO327 may represent the prototype of an entirely new family of high-Tc superconductors, where the straightening out of the Ni-O-Ni bond angle accompanied by the loss of the octahedral tilting is thought playing the main role[1,2]. However, the requirement of relatively high hydrostatic pressure severely limits fundamental investigation of its superconducting state, as most spectroscopic probes are incompatible with such conditions. By exploiting the unique tuning parameters offered by thin-film growth, such as epitaxial strain, dimensional confinement, and interface engineering, significant progress has already been achieved. In late 2025, LNO327 thin films displayed a superconducting transition with a critical temperature below 42 K following ozone annealing3. However, the superconducting phase remains highly elusive, leaving considerable room for further optimization and discoveries.
In this work, we present a detailed structural study of compressively strained LNO327 thin films by using scanning transmission electron microscopy combined with electron energy loss spectroscopy. The films were grown onto (001)-oriented $SrLaAlO_4$ substrates by pulsed laser deposition assisted by reflection high energy electron diffraction. By comparing differently annealed films, resulting in distinct superconducting properties, we show a structural reference framework for LNO327 thin films and highlight the range of structural configurations accessible in this system (LNO-2222 vs LNO-1313), offering new insight into the structure that possibly stabilize superconductivity at ambient pressure and guiding future efforts to engineer more stable superconducting nickelates.

1. Sun, H. et al. Signatures of superconductivity near 80 K in a nickelate under high pressure. Nature 621, 493–498 (2023).
2. Wang, L. et al. Structure Responsible for the Superconducting State in La3Ni2O7 at High-Pressure and Low-Temperature Conditions. J. Am. Chem. Soc. 146, 7506–7514 (2024).
3. Ko, E. K. et al. Signatures of ambient pressure superconductivity in thin film La3Ni2O7. Nature 638, 935–940 (2025).

110	**Electronic Structure of $La_3Ni_2O_7$**	Kun Jiang	Contributed talk (17:30-17:45)

Kun Jiang (1) Yuxin Wang (1) Zhan Wang (1) Fuchun Zhang (2)

(1) Institute of Physics, Chinese Academy of Sciences, Beijing
(2) University of Chinese Academy of Sciences

We present a systematic study of the electronic structure of $La_3Ni_2O_7$, focusing on the roles of the \gamma band, Jahn–Teller (JT) distortion, and apical oxygen vacancies. We show that the γ band is highly sensitive to details of the numerical approximations, and can therefore strongly influence the low-energy electronic states. For thin films, epitaxial strain predominantly enhances the JT splitting between d_{z^2} and $d_{x^2-y^2}$ orbitals, thereby reshaping the Fermi surface, while the interlayer coupling remains comparatively unchanged. In contrast, apical oxygen deficiency significantly reconstructs the band structure by suppressing interlayer hybridization.

206	**Correlated electrons in bilayer nickelates: from $La_3Ni_2O_7$ to $La_3Ni_2O_6$**	Frank Lechermann	Contributed talk (17:45-18:00)

Frank Lechermann (1) Steffen Bötzel (1) Ilya M. Eremin (1) Jannik Gondolf (2)

(1) Ruhr University Bochum
(2) University of Copenhagen

There are two known superconducting nickelate families, i.e. low-valence Ni($3d^{9-\delta}$) compounds and Ruddelsden-Popper (RP) materials with Ni($3d^{8-\delta}$) valence. While both families host NiO_2 square planes, key difference is given by the missing apical oxygen atoms in the low-valence nickelates. A possible route to connect both nickelate families might be given by the reduction of the $La_3Ni_2O_7$ RP bilayer compound, i.e. by removing it's apical oxygens. Complete removal results in the $La_3Ni_2O_6$ compound, while taking out only half of the apical oxygens results in the $La_3Ni_2O_{6.5}$ system. Those reduced materials are so far only scarcely characterized experimentally, but display quite intriguing correlation physics from theory. We will discuss the results of advanced first-principles many body calculations for correlated electrons in the different bilayer nickelates, highlighting variations in the mechanisms at strong coupling as well as the challenging low-temperature physics.

M07 – Session 3 (Wed 23, 16:00-18:00, Chair: Karsten Held)

ID	Title	Speaker	Type
344	**Microscopic origin of superconductivity and stripe magnetism in bilayer nickelates**	Tobias Helbig	Contributed talk (16:00-16:15)

Tobias Helbig (1) Yiming Wu (1) Hanbit Oh (2) Salahudin V. Smailagić (1) Bai Yang Wang (1) Jiarui Li (1) Yijun Yu (1) Harold Y. Hwang (1) Hong-Chen Jiang (1) Srinivas Raghu (1)

(1) Stanford University
(2) Johns Hopkins University

The discovery of the bilayer nickelate $La_3Ni_2O_7$ as a high-temperature superconductor in bulk and thin film samples has raised fundamental questions about the origin of its unusually high transition temperature. While superconductivity emerges at high pressure or compressive strain, the normal state at ambient conditions displays spin stripe order with wavevector $Q = (\pi, 2\pi/2)$. In this talk, we propose a microscopic Hamiltonian that captures the structural evolution from orthorhombic to nearly tetragonal symmetry with increasing pressure, and argue that both stripe magnetism and superconductivity emerge from the interplay of Hund's coupling J_H and interlayer superexchange J_z. Our DMRG calculations show that stripe order arises at sizable J_H from a hidden quasi-one-dimensionality, while superconductivity emerges upon increasing J_z in the crossover between the two regimes. Complementary RPA calculations on a tight-binding model fitted to ARPES data further support the pivotal role of J_H: in the strong Hund's coupling regime $s_{\pm}$-wave pairing dominates over competing d-wave tendencies, while $(\pi, 2\pi/2)$ magnetic ordering is already seeded by Fermi surface nesting at the bare level and further enhanced by J_H.

142	**Theory of density waves in low-pressure $La_3Ni_2O_7$**	Lauro Braz	Contributed talk (16:15-16:30)

Lauro Braz (1) Steffen Bötzel (2) Ilya Eremin (2) Frank Lechermann (2)

(1) Institute of Physics, University of São Paulo
(2) Theoretische Physik III, Ruhr-Universität Bochum

Extensive experimental efforts have been dedicated to understand the low-pressure phase diagram of $La_3Ni_2O_7$ with the ultimate goal of connecting the low-pressure with the high-T_c superconducting high-pressure phase diagram. The bilayer nickelate in its C_4 symmetry-breaking orthorhombic structural phase features a spin-density wave at $T_{SDW} \approx 150$ K and another density wave at $T_{DW} \approx 130$ K. Using unrestricted Hartree-Fock calculations for the single-$\boldsymbol{Q} = (\pi, 0)$ order in the orthorhombic ambient-pressure structure of $La_3Ni_2O_7$, we find that a nematic double-stripe spin-density wave that breaks C_2 symmetry emerges at T_{SDW}, which is followed by a unidirectional charge-density wave at $T_{DW}/T_{SDW} \sim 0.9$ originated from the magnetic fluctuations inside the spin-

density wave state. The charge-density wave is 2-3 orders of magnitude weaker than the spin-density wave and is, therefore, more easily suppressed by external fields or pressure.

509	**Systematic study of trilayer nickelates via ab initio and many-body calculations**	Yuxi Zhang	Contributed talk (16:30-16:45)

Yuxi Zhang (1) Viktor Christiansson (1) Karsten Held (1)

(1) TU Wien

Motivated by the experimental discovery of superconductivity in the trilayer Ruddlesden-Popper nickelate superconductor $La_4Ni_3O_{10}$, we investigate the electronic structure for both the ambient pressure and high pressure phase. A two-orbital three-layer minimum model is constructed from maximally-localized Wannier orbitals of Ni e_g character. Furthermore, systematic dynamical mean-field theory (DMFT) and quantum Monte Carlo (QMC) simulations are performed, where we confirm the picture of orbital-selective correlations and discuss the role of Hund's coupling J, and its competition with the interlayer coupling $t_\perp$ and Hubbard U, in the description of the low-energy correlated electronic structure and pairing tendencies.

119	**Self-doped Molecular Mott Insulator and d-wave Pairing in $La_3Ni_2O_7$**	Zhan Wang	Contributed talk (16:45-17:00)

Zhan Wang (1) Hui-Ke Jin (2) Kun Jiang Fuchun Zhang (1)

(1) Institute of Physics, Chinese Academy of Sciences
(2) ShanghaiTech University
(3) University of Chinese Academy of Sciences

Bilayer nickelate $La_3Ni_2O_7$ offers a new setting to study the interplay between Mottness, multi-orbital physics, and superconductivity. We show that a bilayer Hubbard model supports a molecular Mott state driven by strong interaction and interlayer coupling, which becomes self-doped through charge transfer to higher-energy bands as the interlayer coupling is reduced. Guided by this picture, we study a two-band t-J model and find an orbital-selective d-wave superconducting state emerging only from the itinerant orbital, while the quasi-localized orbital suppresses pairing by promoting local inter-orbital bound states. These results support a picture of $La_3Ni_2O_7$ as a self-doped molecular Mott system and suggest that suppressing localized dz^2-derived states may help enhance superconductivity.

189	**A unified theory for bulk and thin-film bilayer nickelate $La_3Ni_2O_7$**	Jiangfan Wang	Contributed talk (17:00-17:15)

Jiangfan Wang (1) Yi-feng Yang (1)

(1) Institute of Physics, Chinese Academy of Sciences

The discovery of superconductivity in Ruddlesden-Popper bilayer nickelates has drawn enormous attention. We provide a unified theoretical explanation based on the two-component scenario for many experimental observations on bulk and thin film $La_3Ni_2O_7$, including the different superconducting transition temperatures, the nontrivial normal states, the effects of doping, and the Kondo effect in non-superconducting samples. For large interlayer superexchange, our theory predicts two different superconducting domes separated by a valence bond solid state for nearly half-filled d_{z^2} orbital. The breaking of valence bonds by inner apical oxygen vacancies leads to Kondo effect. For small interlayer coupling, superconductivity emerges around half filling with T_c less sensitive to d_{z^2} doping, corresponding to thin films. Upon d_{z^2} doping, the normal state shows a crossover from Fermi liquid to non-Fermi liquid and weak insulating behaviors, consistent with recent experiments. Our theory predicts ambient-pressure superconductivity may emerge in bulk $La_3Ni_2O_7$ by reducing the interlayer magnetic coupling.

155	**Dimensionality of vortex matter in superconducting infinite-layer nickelates**	David Sanchez-Manzano	Contributed talk (17:15-17:30)

David Sanchez-Manzano (1) V. Humbert (2) D. Zhang (2) A. Gutierrez-Llorente (2) M. Bibes (2) J. Santamaria (1) L. Iglesias (2) Javier E. Villegas (2)

(1) Universidad Complutense de Madrid
(2) Laboratoire Albert Fert

Characterizing the dimensionality of the superconducting state in infinite-layer (IL) nickelates is essential for understanding its nature. Most studies have addressed this by examining the anisotropy of the upper critical fields. However, the dominance of Pauli paramagnetic effects over orbital effects complicates the interpretation of these experiments in terms of dimensionality. Here, we approach the question from a different perspective by mapping the vortex phase diagram. We show that superconducting $Pr_{0.8}Sr_{0.2}NiO_2$ thin films with low disorder exhibit a vortex liquid-to-glass transition of a quasi-two-dimensional (2D) nature. In contrast, increasing disorder drives a crossover into a pure 2D state. This demonstrates that pure bidimensionality is an extrinsic property, resulting from the decoupling of NiO_2 planes due to enhanced disorder. Our findings establish disorder as a key control parameter of superconductivity in IL nickelates and suggest that it resides within the NiO_2 planes, providing two fundamental insights for understanding these materials [1].

[1] D. Sanchez-Manzano et al, arXiv:2410.14341 (2026)

618	**Single-band fluorides akin to infinite-layer cuprate superconductors**	Wenfeng Wu	Contributed talk (17:30-17:45)

Wenfeng Wu (1,2) Eric Jacob (3) Viktor Christiansson (3) Ying Gao (4) Zhi Zeng (1,2) Karsten Held (3) Liang Si (3,4)

(1) Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences, Hefei, China
(2) Science Island Branch of Graduate School, University of Science and Technology of China, Hefei, China
(3) Institute of Solid State Physics, TU Wien

(4) School of Physics, Northwest University, Xi'an

Recent experimental discoveries of infinite- and finite-layer nickelate superconductors have highlighted the importance of a single-band $d_{x^2-y^2}$ Fermi surface for enabling unconventional superconductivity similar to cuprates. Motivated by this, we use density functional theory (DFT) and dynamical mean-field theory (DMFT) to identify two infinite-layer fluorides—$KNiF_2$ and $KPdF_2$—as promising candidates. Both materials exhibit strong correlations, structural stability, a single-band $d_{x^2-y^2}$ Fermi surface, and an antiferromagnetic Mott insulating state for the undoped parent compound. However, in $KNiF_2$, overly strong correlations suppress spin fluctuations, preventing the electron pairing and superconducting states at finite temperatures. In contrast, $KPdF_2$ offers tunable superconducting behavior. Using dynamical vertex approximation (DΓA), we show that 20% hole doping on $SrTiO_3$ and 10% electron doping on MgO substrate yield superconducting transition temperatures of 65 K and 63 K, respectively, demonstrating the material's potential through doping and substrate engineering.

471	**Importance of long-range hopping beyond the conventional Emery model for cuprate superconductivity**	Eric Jacob	Contributed talk (17:45-18:00)

Eric Jacob (1) Viktor Christiansson (1) Philipp Hansmann (2) Karsten Held (1) M. O. Malcolms (3) Thomas Schäfer (3) Liang Si (4) Leonard M. Verhoff (1) Paul Worm (1)

(1) TU Wien
(2) Friedrich-Alexander-Universität Erlangen Nürnberg
(3) Max-Planck-Institut für Festkörperforschung
(4) School of Physics, Northwest University (China)

The infinite-layer cuprate superconductors are the prototypical material family for exploring unconventional superconductivity and correlated electronic phenomena. We present a numerical study using the dynamical vertex approximation [1] of a three-band Emery model [2] that goes beyond the one-band Hubbard description. We find (i) a pseudogap [3] and (ii) a strong dependence of the band structure and superconducting dome on long-range hoppings. Neglecting these hoppings shifts the dome and yields a modulated d-wave gap, whereas including them restores a conventional d-wave gap and places the dome in the correct doping range.

[1] G. Rohringer et al., Rev. Mod. Phys. 90, 025003 (2018).
[2] V. J. Emery, Phys. Rev. Lett. 58, 2794 (1987). [3] M. O. Malcolms et al., arXiv:2412.14951 (2024).

Funding by the Austrian Science Fund (FWF) through Grant DOI 10.55776/I5398 (DFG Project No. 465000489) is gratefully acknowledged.

M08 - Superconducting Altermagnets - Fundamentals and Devices

M08 – Session 1 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
167	**Superconductivity in altermagnets: emergent phenomena and constraints**	Annica Black-Schaffer	Invited talk (16:00-16:30)

Annica Black-Schaffer (1)

(1) Uppsala University

Magnetism and superconductivity are two of the most prominent quantum phases of matter, typically exhibiting a competing, “friend–foe” relationship. Their interplay in altermagnets, however, opens a route to qualitatively new phenomena.
In this talk, I will present several effects that arise when superconductivity emerges in altermagnetic systems, including finite-momentum pairing, field-induced superconductivity, and a perfect superconducting diode effect. I will also discuss general constraints imposed by altermagnetism on the superconducting pairing symmetry. If time permits, I will further outline the possibility of orbital-selective altermagnetism in the unconventional superconductor Sr_2RuO_4.

136	**Influencing altermagnetic transitions by strain and layering**	Ilya Eremin	Contributed talk (16:30-16:45)

Ilya Eremin (1) Marnin Di Nunzio (1) Frank Lechermann (1)

(1) Ruhr-Universität Bochum

Altermagnets are collinearly ordered magnets, that break time-reversal symmetry, with a zero magnetization, and a spin-split band structure. By employing the minimal tight-binding Hubbard-like model within mean-field and rotationally invariant slave boson (RISB) approximation we explore the effect of uniaxial strain and electronic correlations on altermagnetism in mono- and bilayer systems. We single out two configurations of bilayer stackings and examine the altermagnetic transition and the effect of doping respectively. Following the application of uniaxial strain and doping in the monolayer, we uncover a fully spin-polarized Fermi surface. In the bilayer system doping itself is sufficient to achieve a complete metallic spin-polarization.

576	**Superconducting Signatures of Altermagnetism: From Critical Anisotropies to Nonreciprocal Vortex Response**	Andrei Mazanik	Contributed talk (16:45-17:00)

Andrei Mazanik (1) Sebastián Bergeret (1) Rodrigo de las Heras (1)

(1) Centro de Física de Materiales (CFM-MPC) Centro Mixto CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain

We present a unified theoretical study of superconducting films and heterostructures hosting collinear d-wave altermagnetic order. Using a Ginzburg-Landau description, we show that the interplay between superconductivity and altermagnetism produces characteristic fourfold anisotropies in the critical temperature, parallel critical field, and critical current density under external magnetic fields and in-plane supercurrents. We further demonstrate that, in the vortex state, altermagnetism transforms conventional circular Abrikosov vortices into elliptical ones, with their orientation controlled by the sign of the magnetic-field component parallel to the Néel vector. As a consequence, superconducting films with pinning defects or geometrical constraints can exhibit nonreciprocal magnetization curves arising from different vortex-vortex interaction energies for opposite field orientations. These effects originate from an altermagnetism-induced effective-mass anisotropy generated by the coupling between the external field and the Néel vector. Together, these results identify a broad set of experimentally accessible superconducting signatures of altermagnetism, relevant both to intrinsic altermagnetic superconductors and to superconductor/altermagnet hybrid structures.

476	**Altermagnetic Thin Films and Their Interplay with Superconductivity**	Dominik Kriegner	Invited talk (17:00-17:30)

Dominik Kriegner (1)

(1) Institute of Physics of the Czech Academy of Sciences

Altermagnets are compensated collinear magnets whose opposite sublattices are related by lattice rotations rather than translations [1]. This symmetry leads to spin-split electronic bands with alternating sign in momentum space despite vanishing net magnetization. We recently demonstrated this band splitting in hexagonal MnTe [2], where it also gives rise to linear response phenomena usually associated with ferromagnets [3].
In this talk I will present our recent progress toward altermagnetic thin films and hybrid structures aimed at superconducting spintronics. First, I will discuss the extension of altermagnetic concepts to sputtered thin films and highlight thin-film materials as a scalable platform for realizing spin-split bands [4], including with a view toward transport signatures such as the anomalous Hall effect. These results establish altermagnetic thin films as a versatile platform beyond bulk model systems. Second, I will show our first steps toward combining altermagnetism with superconductivity. We have recently realized epitaxial superconductor/altermagnet bilayers and are now investigating how superconducting and altermagnetic order interact at the interface [5]. Such heterostructures provide a platform to explore superconducting proximity effects and spin-dependent pairing in spin-split systems without net magnetization.

[1] L. Smejkal, J. Sinova, and T. Jungwirth, Phys. Rev. X 12, 031042 & 040501 (2022).
[2] J. Krempaský et al., Nature 626, 517–522 (2024).
[3] O. J. Amin et al., Nature 636, 348–353 (2024).
[4] S. P. Bommanaboyena et al., Phys. Rev. Materials 9, 064402 (2025).
[5] C. Müller et al., arXiv:2601.06504 [cond-mat.supr-con].

226	**Perfect spin nonreciprocity in gated superconducting altermagnetic heterostructures**	Peihao Fu	Contributed talk (17:30-17:45)

Peihao Fu (1) Luca Chirolli (1) Jorge Cayao (2)

(1) University of Florence
(2) Uppsala University

We consider a superconducting altermagnet heterostructure and demonstrate that the interplay between altermagnetism and a selective filter of transverse momentum channels enables perfect nonreciprocal spin-polarized currents. We demonstrate that this nonreciprocity manifests in both local and nonlocal spin currents, signalling the emergence of directionally selective local and nonlocal spin behaviors. We show that the selective filter of transverse momentum channels is realized by gating a finite normal region between the superconducting altermagnet and the metallic reservoir, which then directionally selects transport channels that match the momentum-dependent spin-split superconducting altermagnetic states and allow nonreciprocal spin-polarized currents. We discover that the local and nonlocal spin nonreciprocity features a highly tunable polarity and nearly perfect and perfect quality factors, respectively, achieved by means of gate voltages and varying the length of the finite region. Moreover, we find that local and nonlocal charge currents also develop a nonreciprocal behavior, whose quality factors can also reach perfect values. In all cases, the spin and charge currents are sensitive to variations of the altermagnetic field, a functional dependence that can be exploited to identify the type of altermagnetism. Our findings put forward an electrically controllable route towards nonreciprocal superconducting spintronic devices based on altermagnets.

469	**Transport in Altermagnet/Superconductor Junctions with Rashba Spin-Orbit Coupling**	František Herman	Contributed talk (17:45-18:00)

Lucia Gelenekyová (1) Andreas Costa (2) Jaroslav Fabian (2,3) František Herman (1)

(1) Comenius University in Bratislava
(2) University of Regensburg
(3) Halle-Berlin-Regensburg Cluster of Excellence CCE

Altermagnets (AMs) [1] have recently emerged as a promising platform in condensed matter physics, with possible applications in multilayer nanostructures such as magnetic superconducting tunnel junctions [2]. Compared with ferromagnets (Fs), which are commonly employed in a similar fashion [3], altermagnets offer the key advantage of vanishing macroscopic magnetization—a property that enhances their compatibility with superconductivity, while still enabling spin-polarized transport.
In this work, we theoretically investigate the transport properties of a three-dimensional vertical tunnel junction comprising semi-infinite AM and s-wave superconductor (S) electrodes; the interface between the two electrodes is modeled as a thin tunneling barrier that induces Rashba spin-orbit coupling (SOC). By computing the conductance spectra of the AM/S junction for realistic parameter regimes and for different orientations of the spin-split altermagnetic Fermi surfaces relative to the interface, we identify experimentally accessible signatures to map the conductance features to the underlying Fermi-surface structure of the AM.
Furthermore, we analyze unconventional Andreev reflections at the interface, which can generate a spin-polarized triplet supercurrent in the intrinsically singlet s-wave S mediated by SOC-induced spin flips. We examine the angular dependence of these unconventional Andreev reflections—and consequently, the efficiency of triplet-pair generation—upon rotating the spin-split Fermi surfaces with respect to the interface. Our results are finally contrasted with the well-established behavior of ferromagnetic F/S junctions [3].

[1] L. Šmejkal, J. Sinova, T. Jungwirth, Emerging Research Landscape of Altermagnetism, Phys. Rev. X 12, 040501 (2022).
[2] M. Papaj, Andreev reflection at the altermagnet-superconductor interface, Phys. Rev. B 108, L060508 (2023), and the references therein.
[3] P. Högl, A. Matos-Abiague, I. Žutić, J. Fabian, Magnetoanisotropic Andreev Reflection in Ferromagnet-Superconductor Junctions, Phys. Rev. Lett. 115, 116601 (2015).

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M08 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
220 **P005**	**From pure to mixed altermagnets: A study of Sr_2RuO_4 and Sr_2IrO_4**	Jabed Umar	Poster

Jabed Umar (1) Aline Ramires (1)

(1) Technische Universität Wien

Altermagnetism has recently emerged as a distinct magnetic phase with strong potential for spintronic applications, characterized by momentum-dependent spin splitting in the absence of net magnetization [PhysRevX.12.040501]. In real materials, the presence of unavoidable spin–orbit coupling (SOC) further enriches this picture. Recent studies [PhysRevB.109.024404] have shown that the presence or absence of an anomalous Hall effect (AHE) distinguishes two types of altermagnets: mixed and pure altermagnets, a classification rooted in the irreducible representations (irreps) of the point group of the underlying crystal. When the altermagnetic order parameter and a Hall vector transform according to the same irreps, they can coexist in superposition, giving rise to a mixed altermagnetic phase with a finite AHE; otherwise, the phase remains purely altermagnetic.
Motivated by this framework, we investigate the evolution from pure to mixed altermagnetic behavior in two paradigmatic layered oxides, Sr_2RuO_4 and Sr_2IrO_4. In Sr_2RuO_4 , the surface of RuO_6 octahedra has C_{4v} point group, a collinear compensated magnetic order with moments polarized along the axis transforms as a pure altermagnet, which is symmetry-incompatible with a Hall vector and therefore does not generate an AHE. Importantly, additional symmetry lowering—arising from strain, or secondary electronic orders—can transmute the nominally pure z-polarized altermagnetic state into a mixed one, thereby enabling a finite AHE.
By comparison, Sr_2IrO_4 exhibits a more intricate situation. Depending on the stacking of single or multiple IrO_6 layers, the allowed magnetic order parameters transform according to different irrps, permitting both pure and mixed altermagnetic phases. Through symmetry analysis, we show how structural distortion or other secondary orders govern the transition from pure to mixed altermagnetism, and outline experimental signatures in transport measurements. Our

results identify layered ruthenates and iridates as fertile ground for realizing and tuning altermagnetic phenomena, and suggest concrete pathways for engineering altermagnetism in correlated materials and future quantum technologies.

499 **P006**	**Sublattice Degrees of Freedom and Non-Unitary Pairing in Altermagnetic Superconductors**	Christian Lukas Hestbjerg Rasmussen	Poster

Christian Lukas Hestbjerg Rasmussen (1)

(1) Niels Bohr Institute, University of Copenhagen

In this talk, I address the fundamental question of how the superconducting state is defined in altermagnetic metals. Although these systems are characterized by spin-split Fermi surfaces and a compensated Néel-type magnetic order, the microscopic nature and symmetry classification of their superconducting instabilities remain incompletely understood.
Employing realistic microscopic models that explicitly resolve the essential altermagnetic sublattice degrees of freedom, I demonstrate that the sublattice structure constitutes a primary controlling factor of the superconducting gap topology. Specifically, for superconducting states stabilized by momentum-independent bare attractive interactions, I find that the underlying symmetry of the altermagnetic lattice rigorously enforces gap nodes at the Brillouin-zone boundaries.
I subsequently contrast these results with the case of superconductivity arising from extended-range interactions. In this regime, I demonstrate that Cooper pairing is allowed on the Brillouin-zone boundaries, which enables the stabilization of both spin-singlet and equal-spin-pairing triplet superconducting states. A principal conclusion of this study is that equal-spin-pairing triplet superconductivity is generically energetically favored when the altermagnetic spin splitting of the electronic bands is large compared to the characteristic superconducting gap scale.
Finally, I will discuss how these triplet states feature characteristic non-unitary properties that arise as a direct consequence of the altermagnetic order. By focusing on the interplay between sublattice degrees of freedom and pairing symmetry, I provide a theoretical framework for identifying these unconventional states in candidate altermagnetic materials.

520 **P007**	**Exotic vortex states within chiral superconducting states**	Frederik Alexander Stege Philipsen	Poster

Frederik Alexander Stege Philipsen (1)

(1) University of Copenhagen

Motivated by experimental developments reporting evidence of time-reversal symmetry breaking in the superconducting state of kagome metals, an investigation into the nature of vortices in chiral $d + id$ superconductors on the kagome lattice will be presented. Using self-consistent microscopic calculations that incorporate the band structure characteristics of the kagome lattice, the ground-state condensate in the presence of an external field was found to host fractional vortices. Each fractional vortex carries one-third of the superconducting flux quantum and exhibits a characteristic signature related to one of the three sublattice degrees of freedom of the kagome lattice. Extending these calculations to the altermagnetic bipartite square lattice, the vortex state of the four-fold degenerate chiral equal-spin pairing $p + ip$-wave state is explored. With the decoupling of the two spin condensates in addition to the chiral order of the individual condensates, this system offers a wide range of possibilities for the realization of fractional vortex states.

431 **P008**	**Fragility of the Magnetic Order in the Prototypical Altermagnet RuO_2**	Andriy Smolyanyuk	Poster

Andriy Smolyanyuk (1) Laura Garcia-Gassull (2) Igor I. Mazin (3) Roser Valenti (2) Libor Šmejkal (4)

(1) TU Wien, Institute of Solid State Physics
(2) Goethe-Universität Frankfurt
(3) George Mason University
(4) Max Planck Institute for the Physics of Complex Systems

Altermagnetism is a topic that has recently been gaining attention, and the RuO_2 compound is among the most studied altermagnetic candidates. However, a survey of the available literature on RuO_2 properties suggests no consensus on its magnetism. By performing density functional theory (DFT) calculations, we show that the electronic properties of stoichiometric RuO_2 are described in terms of a Hubbard U, within DFT+U, smaller than the value required to have magnetism. We further argue that Ru vacancies can actually aid the formation of a magnetic state in RuO_2. This, in turn, suggests that a characterization of the amount of Ru vacancies in experimental samples might help resolve the controversy between the different experimental results.
The electronic structure of RuO_2 hints at a possibility of realizing a magnetically ordered state upon hole doping, and such a possibility was explored experimentally in Cr-doped RuO_2, where it was suggested that this system exhibits the anomalous Hall effect (AHE) due to altermagnetism. Based on our density functional calculations, we revise the results obtained for this system and propose a different interpretation of experimental results. Our calculations suggest that extra holes are bound to the Cr impurity and do not dope the Ru bands, which remain nonmagnetic. Thus, the observed AHE is not due to the altermagnetism but stems entirely from magnetic Cr ions.

M09 - Magnetism and Superconductivity in Nanoscale 3D Architectures

M09 – Session 1 (Tue 22, 10:30-12:30, Chairs: Claas Abert and Amalio Fernandez-Pacheco)			
ID	Title	Speaker	Type
125	**From Quantum Rings to 3D Nanoarchitectures: Effects of Geometry and Topology**	Vladimir M. Fomin	Invited talk (10:30-11:00)

Vladimir M. Fomin (1,2)

(1) Leibniz Institute for Solid State and Materials Research (IFW) Dresden, Germany
(2) Moldova State University, Chişinău, Republic of Moldova

State-of-the art fabrication techniques allow for creation of topologically non-trivial and geometrically complex nanostructures ranging from quantum rings to 3D nanoarchitectures. Quantum rings are a special class of high-tech nanostructures, which provide a unique playground for the quantum-mechanical paradigm and topological physics [1]. Models of magnetoresistance oscillations in mesoscopic rings of low- and high-critical-temperature superconductors take into account the quantum-interference manifestations. Self-assembly and direct writing of 3D nanoarchitectures trigger the emergence of new physical phenomena [2]. In superconductor open nanotubes and nanohelices, a topological transition between the vortex and phase-slip regimes determines the magnetic-fieldvoltage and currentvoltage characteristics revealing a nontrivial topology of superconducting screening currents. In a densely packed WC nanoarray fabricated using FIBID [3], in addition to vortex pinning, periodic magnetoresistance oscillations may be associated with magnetic flux quantization effects and interference of circulating supercurrents within the periodic structure. In a directly written superconductor WC nanobridge, a strong anisotropy of the critical magnetic field gives rise to the reconfigurable coexistence of superconducting and normal states. In this regime of nano-superconductivity, the vortex state can be designed and manipulated by geometric confinement [4]. These findings highlight the potential of 3D nanoarchitectures as a prospective platform for quantum technologies [5].

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A. Arroyo-Fructuoso et al., APL Quantum 3, 016108 (2026).
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O. Dobrovolskiy et al., Supercond. Sci. Technol. 39, 023502 (2026).

82	**Unconventional Josephson Supercurrent Diode Effect Induced by Chiral Spin-Orbit Coupling**	Andreas Costa	Contributed talk (11:00-11:15)

Andreas Costa (1) Osamu Kanehira (2) Hiroaki Matsueda (2) Jaroslav Fabian (1,3)

(1) University of Regensburg, Germany
(2) Tohoku University, Japan
(3) Halle-Berlin-Regensburg Cluster of Excellence CCE, Germany

First-principles calculations have recently predicted that chiral materials lacking mirror symmetries---such as twisted van-der-Waals homobilayers---can feature unconventional radial Rashba coupling with spins aligned fully parallel (instead of tangentially) to momentum.
In this talk, we will address Josephson transport through vertical superconductor/ferromagnet/superconductor junctions hosting crossed (radial and tangential) Rashba fields at the interfaces and demonstrate that their interplay with ferromagnetic exchange can lead to supercurrent rectification even when the magnetization is collinear with the current. This so-called unconventional supercurrent diode effect (SDE) originates from spin precessions inside the ferromagnet, which imprint polarity-dependent transmission probabilities on the Cooper pairs being well-distinct from the conventional SDE, and provides a sensitive probe of chiral spin textures.

This work has been supported by Deutsche Forschungsgemeinschaft (DFG; German Research Foundation)---Projects 454646522; 314695032 (SFB 1277).

96	**Focused Ion Beam Nanofabrication of 3D Nanosuperconductors and Devices**	Rosa Córdoba	Contributed talk (11:15-11:30)

Rosa Córdoba (1) A. Arroyo-Fructuoso (1) R. Huebner (2) G. Hlawacek (2) V. M. Fomin (3)

(1) Institute of Molecular Science (ICMol), University of Valencia, Paterna, Spain
(2) Ion Beam Center, Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany
(3) Institute for Integrative Nanosciences, Dresden, Germany

Superconducting nanostructures are attractive building blocks for future quantum and nanoelectronic technologies because they combine dissipationless transport, macroscopic quantum coherence, and strong sensitivity to geometry and dimensionality. In particular, extending superconductivity from planar systems to three-dimensional (3D) nanoscale architectures creates new opportunities to tailor electronic, magnetic, and optical functionalities through structural design.
Here we present a direct-write additive nanofabrication approach based on focused ion beam induced deposition for the realization of complex 3D superconducting nanostructures with nanoscale precision. This method enables the controlled growth of free-form geometries, including nanohelices, whose properties can be tuned through their shape, dimensions, and orientation. The fabricated nanohelices exhibit superconductivity with critical temperatures around 7 K and remain robust under high magnetic fields, up to 15 T depending on the field orientation relative to the helical axis, while displaying non-trivial transport behaviour linked to their 3D geometry.
Beyond single nanostructures, we show that geometry engineering provides access to additional functionalities. Chiral 3D superconducting nanoarchitectures display enhanced light–matter interaction, with strong circular dichroism and large dissymmetry factors compared with planar counterparts. In parallel, densely packed planar superconducting nanostructures exhibit enhanced vortex pinning, evidenced by resistance minima at well-defined magnetic fields associated with commensurability effects between the vortex lattice and the artificial geometry. We also demonstrate that the superconducting response of nanowires can be modulated by external electric fields, highlighting the possibility of actively tunable superconducting nanoelements.
Overall, these results establish focused ion beam direct-write nanofabrication as a versatile platform for designing advanced nanosuperconductors in which superconductivity, 3D geometry, chirality, and field tunability can be combined within a single nanoscale system.

128	**Control of topological states and magnetization dynamics on curved surfaces**	Sabri Koraltan	Invited talk (11:30-12:00)

Sabri Koraltan (1)

(1) Institute of Applied Physics, Technische Universität Wien

The extension of nanomagnetism into three dimensions and curvilinear geometries opens new frontiers for spintronic applications, offering additional degrees of freedom beyond conventional planar thin films [1]. This talk presents recent advances in understanding and controlling topological magnetic states such as skyrmions and vortices on curved surfaces.
In the first part of my talk, I will show how the curvature can indirectly assist skyrmion formation on self-assembled polystyrene particles coated with Pt/Co/Ta multilayers [2]. Using magnetic force microscopy (MFM), we demonstrate that the confined spiraling 3D stripe states can be transformed into metastable skyrmions at the apex of spherical particles through local magnetic field stimuli from the MFM tip, despite negligible curvature induced DMI.
On the other hand, spin waves in magnonic systems offer energy-efficient alternatives to conventional electronics [3], with low-frequency magnetic vortex resonances being particularly relevant for microwave applications. While planar magnetic vortices have been extensively studied, their dynamics in three-dimensional curvilinear architectures remain largely unexplored.
In the second part of my talk, I will focus on our latest results on the direct experimental observation of vortex core gyration on a 3D curvilinear surface [4]. Using a stripline antenna on a SiN membrane, we excite self-assembled polystyrene spheres coated with NiFe, which host a vortex lattice state at remanence. Time-resolved scanning transmission X-ray microscopy (TR-STXM) at BESSY II [5] captures real-space, time-resolved dynamics, revealing complex spin-wave modes due to curvature-induced field gradients.

[1] Fernández-Pacheco, A. et al. Nature Communications 8, 15756 (2017).
[2] Koraltan, S. et al. arXiv:2511.22557 (2025).
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396	**Geometry-Controlled Domain Wall Evolution in 3D Spiral Nanowires**	Le Zhao	Contributed talk (12:00-12:15)

Le Zhao (1) Alberto Anadón (2) Amalio Fernandez-Pacheco (1) Anna Mandziak (3) Jakub Mateusz Jurczyk (1) Paweł Nita (3) Marcin Szpytma (3) Michael Walser (1)

(1) TU Wien
(2) CSIC-Universidad de Zaragoza
(3) SOLARIS Synchrotron light Sources

Three-dimensional (3D) magnetic nanostructures provide a versatile platform for exploring magnetization processes governed by geometry and topology beyond planar systems [1-3]. In particular, spiral nanowires represent a typical system in which curvature and local structural variations can strongly influence magnetic domain wall nucleation and dynamics [4-5].
In this work, we investigate FEBID-fabricated 3D spiral nanowires using shadow X-ray magnetic circular dichroism photoemission electron microscopy (XMCD-PEEM). By applying in-plane magnetic fields with different orientations and sequences, we systematically control the nucleation and evolution of magnetic domains in the spirals. Due to the geometrical constraints of the spiral structure, domain walls nucleate at well-defined locations where the local wire orientation becomes perpendicular to the applied magnetic field. By changing the field direction, the nucleation position along the spiral can therefore be tuned. In addition, the local slope of the 3D structure modifies the effective cross-section during thin-film deposition, leading to spatial variations in film thickness. Such geometrically induced thickness gradients modulate local magnetic parameters, including effective anisotropy and domain wall energy. As a result, the 3D geometry defines a complex magnetic energy landscape that governs the evolution of domain walls under applied magnetic fields.
The measurements reveal a range of geometry-driven behaviors, including domain wall automotion, local pinning, and interactions between domain walls. These results highlight the potential of engineered 3D magnetic nanostructures as platforms for controlling domain wall dynamics and for developing functional 3D spintronic architectures.

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[2] APL Mater. 8, 010701 (2020).
[3] J. Phys.: Condens. Matter 37, 143502 (2025).
[4] Sci. Rep. 3, 1492 (2013).
[5] ACS Nano 16, 8860 (2022).

590	**Generation of Bloch Points with Controlled Spin Texture Using Geometrical Boundary Conditions**	Naëmi Leo	Contributed talk (12:15-12:30)

Naëmi Leo (1) Daniel Wolf (2) Alicia Estela Herguedas Alonso (3) Oleksandr Zaiets (2) Jakub Jurczyk (4) Takeaki Gokita (4) John Fullerton (5) Dedalo Sanz-Hernandez (6) Claire Donnelly (7) Andrea Sorrentino (8) Eva Pereiro (8) Lucia Aballe (8) Peter Fisher (9) Rachid Belkhou (10) Claas Abert (11) Dieter Suess (11) Axel Lubk (2) Aurelio Hierro-Rodriguez (3) Amalio Fernandez-Pacheco (4)

(1) Loughborough University, (2) IWF Dresden, (3) Universidad de Oviedo, (4) TU Wien, (5) Argonne National Laboratory, (6) Laboratoire Albert Fert, CNRS, (7) University of Cambridge, (8) ALBA Synchrotron Light Source, (9) Lawrence Berkeley National Laboratory, (10) Synchrotron SOLEIL, (11) University of Vienna

Bloch points are three-dimensional singularities in magnetization that play a key role in topological transformations of spin textures. Using a geometrical approach, here we demonstrate deterministic control of the internal magnetic structure of Bloch point. This is achieved by creating a chirality interface between two three-dimensional double-helix nanowires of opposite helicity, which form a kinked, non-collinear structure. A saturating magnetic field nucleates head-to-head or tail-to-tail configurations at the chirality interface, leading to the formation of a Bloch point in the vicinity of the chirality interface. Combining advanced experimental tomography techniques, including transmission electron microscopy (TEM) and x-ray magnetic circular dichroism (XMCD), with micromagnetic simulations, we confirm that domain walls containing circulating Bloch points are reliably nucleated with predefined polarity and circulation. These Bloch points also have a hyperbolic character, with a helicity angle ≠90°. Due to the combination of tailored geometry and the robustness of the initialization field protocol, our approach thus facilitates future 3D spintronic device architectures containing Bloch points with controlled properties.

M09 – Poster session (PS1 Mon21-Tue22)			
ID	Title	Presenter	Type
246 **P009**	**Synthesis of 3D curved superconducting microstructures by atomic layer deposition of NbN**	Maria Mihaescu	Poster

Dirk Grundler (1) Maria Mihaescu (1)

(1) EPFL

Recent advances in nanofabrication enable three-dimensional (3D) nanoarchitectures for studying curvature-controlled superconductivity [1] which promise unconventional transport characteristics [2]. In this work, we investigate how curvature affects superconducting properties of thin-film NbN using a fabrication approach combining two-photon lithography (TPL) and Plasma-Enhanced Atomic Layer Deposition (PEALD). This additive manufacturing strategy, previously applied to curved ferromagnetic systems [3,4], is extended to superconductors to enable systematic experimental studies of 3D geometry-driven effects. Bow-shaped free-standing polymer structures were fabricated via TPL and coated with 30-nm-thick NbN by PEALD. Cross-sectional analysis using xenon plasma focused ion beam milling and scanning electron microscopy confirms conformal NbN deposition. The film indeed replicates template irregularities resulting from a non-optimized stepwise TPL exposure and further template modification attributed to the deposition process. A thermal treatment of the polymer at 450 °C [2] smoothened the TPL resist surface being preserved in the PEALD. Transport measurements were performed on NbN microbridges on planar Si substrates as well as stepped and curved templates. Planar NbN films exhibited superconductivity with a critical temperature (Tc) of almost 13 K. The growth over rough steps etched into a Si substrate reduced Tc locally to 7.5 K, highlighting sensitivity to morphology. 3D curved microbridges were several micrometres long and exhibited large surface corrugation due to non-optimized templates. Contacted in a four-probe configuration, their transport characteristics indicated the existence of segments which remained normal conducting down to 1.8 K. Measurements of smoothened 3D bridges are in progress. In conclusion, we present a scalable platform for both fabricating 3D NbN nanoarchitectures and exploring experimentally curvature-controlled superconductivity.

[1] V. M. Fomin and O. V. Dobrovolskiy, Appl. Phys. Lett. 120, 090501 (2022).
[2] A. J. M. Deenen and D. Grundler, Nano Lett. DOI: 10.1021/acs.nanolett.5c06341.
[3] H. Guo et al., Adv. Mater. 35, 2303292 (2023). [4] M. Xu et al., Nat. Nanotechnol. 20, 1258–1265 (2026).

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M10 - Mesoscopic Superconductivity and Quantum Circuits

M10 – Session 1 (Mon 21, 10:30-12:30)			
ID	Title	Speaker	Type
783	**Fluxonium qubits: fabrication, control, and a path to scale**	Christian Schneider	Invited talk (10:30-11:00)

C. Schneider (1,2) J. Schirk (1,2) F. Wallner (1,2) N. Bruckmoser (1,2) L. Huang (1,2) M. Zetzl (1,2) S. Filipp (1,2)

(1) Technical University of Munich, School of Natural Sciences, Department of Physics, 85748 Garching, Germany
(2) Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 86748 Garching, Germany

The fluxonium qubit, a small Josephson junction shunted by a superinductance, offers large anharmonicity, protection from charge noise, and coherence times beyond the millisecond, making it a compelling alternative to the transmon. I will present our recent progress in developing fluxonium as a scalable platform. First, I will discuss improvements in our junction fabrication process, benchmarked using junction-array resonators that probe array uniformity and internal losses and feed back directly into process development. I will then present results on single-qubit control, including calibration strategies adapted to fluxonium's rich level structure. Finally, I will show early results on multi-qubit devices and discuss the architectural choices that make fluxonium a credible candidate for scaling.

343	**Longitudinal qubit readout from Jaynes-Cummings coupling and strong drive**	Luciano Pereira	Contributed talk (11:00-11:15)

Juan Jose Garcia-Ripoll (1) Luciano Pereira (2) Tomas Ramos (1)

(1) IFF-CSIC Madrid
(2) ICFO-Institut de Ciencies Fotoniques

In superconducting qubits, the standard measurement strategy is dispersive readout, where the qubit is coupled to an off-resonant cavity via a Jaynes-Cummings coupling [1]. This readout scheme works well for weak readout pulses, but its fidelity diminishes when the readout strength exceeds a critical value [2] due to measurement-induced state transitions [3].
Here, we introduce a new dispersive qubit readout scheme specially designed for strong readout pulses. By applying a specific pulse shape, we can correct non-QND features, inducing an effective longitudinal readout despite the qubit-cavity coupling being of the Jaynes-Cummings type. Based on exact stochastic numerical simulations of the qubit measurement dynamics [4], we demonstrate that the proposed protocol achieves high fidelity and QND-ness at moderate driving strengths, ultimately limited by finite qubit decay. Furthermore, we show numerically that the scheme mitigates non-dispersive errors in state-of-the-art transmon readout, such that the measurement becomes fundamentally limited by leakage to higher levels and beyond-rotating-wave effects.

[1] A. Blais, A. L. Grimsmo, S. M. Girvin, and A. Wallraff, “Circuit quantum electrodynamics”, Mod. Rev. Phys. 93, 025005 (2021).
[2] T. Walter et al., "Rapid High-Fidelity Single-Shot Dispersive Readout of Superconducting Qubits", Phys. Rev. Applied 7, 054020 (2017).
[3] M. F. Dumas et al., “Measurement-Induced Transmon Ionization”, Phys. Rev. X 14, 041023 (2024).
[4] L. Pereira, J.J. García-Ripoll, T. Ramos, “Complete physical characterization of QND measurements via tomography”, Phys. Rev. Lett. 129, 010402 (2022).

229	**High fidelity at high power and suppression of measurement induced state transitions in transmon readout using a non-linear coupling**	Olivier Buisson	Invited talk (11:15-11:45)

Cyril Mori (1) Francesca D'Esposito (1) Alexandru Petrescu (2) Lucas Ruela (1) Vladimir Milchakov (1) Olivier Buisson (1) Wael Ardati (1) Dorian Nicolas (1) Vishnu Suresh (1) Shelender Kumar (1) Martina Esposito (1) Gwenael Le Gal (1) Giulio Cappelli (1) Arpit Ranadive (1) Thomas Ramos (3) Quentin Ficheux (1) Nicolas Roch (1)

(1) Institut NEEL-CNRS-UGA-France
(2) Laboratoire de Physique de l’Ecole Normale Supérieure, Inria, ENS, Mines ParisTech, Université PSL, Sorbonne Université, Paris, France
(3) IFF-CSIC-Madrid-Spain

The field of superconducting qubits is constantly evolving with new types of circuit and designs but, when it comes to qubit readout, the use of simple transverse linear coupling is overwhelmingly prevalent. This type of coupling intrinsically limits the readout mode’s dispersive shift and is known to cause Purcell effect. We propose here to overcome these limitations by engineering a non-linear cosϕ-coupling between the transmon qubit and a dedicated readout mode. This is based upon previous published work [1] on qubit readout with a non-perturbative cross-Kerr coupling engineered by a transmon molecule circuit. A new sample with optimized design and parameters shows a readout fidelity of 99.21% measured using a parametric amplifier and a high Quantum Non- Demolition (QND) fidelity of 97% [2]. Interestingly, these results have been achieved with 89 photons in the readout mode. In addition, we have observed suppression of measurement-induced state transitions (MIST) up to high photon counts above 300 [3]. This effect can be explained by the symmetry of the coupling, which is tunable with a magnetic field. All of these measurements were corroborated by a theoretical study, a numerical analysis of the spectra associated with the nonlinearly coupled circuit, and simulations of the corresponding classical dynamics [3]. In conclusion, we show that the cosϕ-coupling is more robust to measurement photons than the usual linear coupling, making it a compelling alternative for high fidelity and non-destructive transmon readout.

[1] R. Dassonneville, et al., “Fast high-fidelity quantum non-demolition qubit readout via a nonperturbative cross-Kerr coupling”, Phys. Rev. X 10, 011045 (2020).
[2] C. Mori, et al., “High-power readout of a transmon qubit using a nonlinear coupling”, arXiv 2507.03642 (2025).
[3] C. Mori, et al., “Suppression of measurement-induced state transitions in cosϕ-coupling transmon readout”, arXiv 2509.05126 (2025).

508	**Infrared-Induced Quasiparticles in Superconducting Qubits**	Felix Wagner	Contributed talk (11:45-12:00)

Felix Wagner (1)

(1) ETH Zurich

Superconducting qubits are one of the most promising platforms for universal quantum computing, yet they suffer from errors induced by interactions with their environment. In particular, radiation — both in the high-energy and infrared regimes — can break Cooper pairs in the superconductor and create Bogoliubov quasiparticles. Upon diffusing towards the Josephson junction, these quasiparticles can tunnel through its insulating barrier, causing energy and phase errors in the process. While this poses a challenge for the resilience of quantum computers, it simultaneously presents an opportunity to exploit this extreme environmental sensitivity for quantum sensing applications in fundamental physics.
In this talk, we will review our work on the interaction of infrared radiation with tantalum- and niobium-based superconducting qubits, as well as mitigation strategies. We will further present a setup employing a quantum cascade laser in the THz regime, designed to characterize the time-resolved response of our devices to infrared radiation bursts. This approach is useful both for studying qubit decay channels and for characterizing these devices as quasiparticle sensors.

450	**Pure dephasing of superconducting qubits due to Bogolyubov quasiparticles tunneling**	Kirill Dubovitskii	Contributed talk (12:00-12:15)

Kirill Dubovitskii (1) Denis Basko (2) Manuel Houzet (3,4) Julia Meyer (3,4)

(1) Inria, Paris
(2) Université Grenoble Alpes, Laboratoire de Physique et Modelisation des Milieux Condensés, CNRS, Grenoble
(3) Université Grenoble Alpes, IRIG-PHELIQS, Grenoble, France
(4) CEA, INAC-PHELIQS, Grenoble

Bogolyubov quasiparticles represent an important sources of errors in superconducting qubits. Unlike the quasiparticle contribution to $1/T_1$ qubit relaxation rate, the pure dephasing rate $1/T_\phi$ can not be obtained by the perturbative golden rule calculation due to the logarithmic divergence of the quasiparticle noise correlator at low frequency (1). For such noises with a divergent correlator, non-perturbative calculations usually reveal a non-exponential decay of the qubit coherence. Particularly, for the quasiparticles in the work (2) the dephasing function of the form $F(t) = \exp[-t\log(tT)]$ was found for qubits based on Josephson junctions with a large number of transmission channels N at temperature T. We treat this problem for a finite number of channels and find that the exponential form of the decay is restored at large times. Instead of expanding in the coupling strength or inverse number of channels $1/N$ we take advantage of the low quasiparticle concentration $x_{qp} \ll 1$ and use it a small parameter. In this case the fermionic nature of the quasiparticle bath becomes important; it can be handled using Levitov formula (3), which allows to rewrite the dephasing function $F(t)$ as a determinant of single-particle operators. We find that the non-exponential decay of the dephasing function $F(t)$ described in (2) is followed by the longest-time exponential regime. It is governed by the energy scale of the depth of the Andreev bound states ϵ_A in the Josephson junction, namely $F(t) = \exp[-t\log(T/\epsilon_A)]$ for $t \gg 1/\epsilon_A$. Our results are especially relevant for qubits built on medium- or small-area junctions for which the time scale $1/\epsilon_A$ is comparable to the qubit lifetimes.

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(2) S. Zanker and M. Marthaler, Phys. Rev. B 91, 174504 (2015).
(3) I. Klich ,arXiv:cond-mat/0209642 (cond-mat.mes-hall) (2002).

272	**Proximity effects in gap-engineered superconducting qubits**	Giampiero Marchegiani	Contributed talk (12:15-12:30)

Giampiero Marchegiani (1) Gianluigi Catelani (1,2)

(1) Technology Innovation Institute
(2) Juelich Research Center

Bogoliubov quasiparticles are an intrinsic source of errors for superconducting qubits [1]. These excitations harm the qubit coherence in two ways: i) they can exchange energy with the qubit when tunneling across the junction, and ii) dynamically lead to dephasing, for instance during burst events, by reducing the Josephson energy and so the qubit frequency. In qubits with gap-asymmetric junctions tunnelling-related errors can be efficiently suppressed at low temperatures [2, 3, 4]. Moreover, gap-engineered qubits can provide a probe to study nonequilibrium quasiparticle distributions [3, 5, 6, 7]. In this presentation, we discuss the impact of the proximity effect, absent for gap-symmetric films, on gap-engineered qubits. The proximity effect between the two superconducting layers produces deviations from the ideal BCS density of states (DoS). In particular, a single gap characterizes the two films, with “subgap” states in the higher order parameter film, and broadening of the BCS divergences. The modified DoSs in the two films determine a weaker suppression of the transition rates with decreasing temperature. Moreover, the diverging relaxation rate for qubit transition energy resonant to gap asymmetry is regularized by the proximity effect, and so the related discontinuity in the frequency shift.

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[2] G. Marchegiani, L. Amico, G. Catelani, PRX Quantum 3, 040338 (2022)
[3] T. Connolly, P.D. Kurilovich, S. Diamond, H. Nho, C. G. L. Bøttcher, L. I. Glazman, V. Fatemi, and M. H. Devoret, Phys. Rev. Lett. 132, 217001 (2024)
[4] M. McEwen, K. C. Miao, J. Atalaya, et. al, Phys. Rev. Lett. 133, 240601 (2024)
[5] S. Diamond, V. Fatemi, M. Hays, et. al., PRX Quantum 3, 040304 (2022)
[6] G. Marchegiani, G. Catelani, Commun. Phys. 8, 120 (2025)
[7] D. S. Antonenko, P. D. Kurilovich, F. J. Matute-Canadas, L. I. Glazman, Phys. Rev. B 113, 054504 (2026)

M10 – Session 2 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
83	**Surface Code hardware hamiltonian**	Mohammad Ansari	Invited talk (16:00-16:30)

John Martinis (1) Xuexin Xu (2) Chloé Vignes (3) Kuljeet Kaur (2) Mohammad Ansari (2)

(1) University of California Santa Barbara
(2) Forschungszentrum Jülich
(3) Massachusetts Institute of Technology

In this talk I'll present an overview over the modelling quantum circuits trajectory from pairwise interactions era to modern circuit QED analysis that enables simulating many-body interactions in surface-code quantum processor units (QPUs). Combining a concise diagrammatic formalism with high-precision numerical methods, our approach efficiently evaluates high-order, long-range Pauli string couplings and maps complete chip layouts onto exact effective Hamiltonians. Applying this method to surface-code architectures, such as Google's Sycamore lattice, we identify three distinct operational regimes: computationally stable, error-dominated, and hierarchy-inverted. Our analysis reveals that even modest increases in residual qubit–qubit crosstalk can invert the interaction hierarchy, driving the system from a computationally favorable phase into a topologically ordered regime. This framework thus serves as a powerful guide for optimizing next-generation high-fidelity surface-code hardware and provides a pathway to investigate emergent quantum many-body phenomena.

61	**Ultrafast Single Qubit Gates through Multi-Photon Transition Removal**	Yuan Gao	Contributed talk (16:30-16:45)

Yuan Gao (1) Asier Galicia (1) José Da Costa Jesus (2) Yebin Liu (1) Yorgo Haddad (1) Dmitriy Volkov (1) Jéferson Guimarães (1) Harsh Bhardwaj (1) Markus Jerger (1) Marc Neis (1) Boxi Li (2) Francisco Cárdenas López (2) Felix Motzoi (2) Pavel Bushev (1) Rami Barends (1)

Forschungszentrum Jülich PGI-13
Forschungszentrum Jülich PGI-8

One of the main enablers in quantum computing is having qubit control that is precise and fast. However, qubits typically have multilevel structures making them prone to unwanted transitions from fast gates. This leakage out of the computational subspace is especially detrimental to algorithms as it has been observed to cause long-lived errors, such as in quantum error correction. This forces a choice between either achieving fast gates or having low leakage. Previous works focus on suppressing leakage by mitigating the first to second excited state transition, overlooking multi-photon transitions, and achieving faster gates with further reductions in leakage has remained elusive. Here, we demonstrate single qubit gates with a total leakage error consistently below 2.0×10^{-5}, and obtain fidelities above 99.98% for pulse durations down to 6.8 ns for both X and X/2 gates. This is achieved by removing direct transitions beyond nearest-neighbor levels using a double recursive implementation of the Derivative Removal by Adiabatic Gate (DRAG) method, which we name the R2D method. Moreover, we find that at such short gate durations and strong driving strengths the main error source is from these higher order transitions. This is all shown in the widely-used superconducting transmon qubit, which has a weakly anharmonic level structure and suffers from higher order transitions significantly. We also introduce an approach for amplifying leakage error that can precisely quantify leakage rates below 10^{-6}. The presented approach can be readily applied to other qubit types as well.

35	**Lattice field theory for superconducting circuits**	Neill Warrington	Contributed talk (16:45-17:00)

Neill Warrington (1)

(1) MIT

Accurately predicting the properties of many-node superconducting circuits devices from circuit QED is challenging as it requires solving the many-body Schrodinger equation. In this talk I will present a new, general method for solving general circuit QED based on lattice field theory, a tool commonly applied in nuclear and particle physics. This method is competitive with state-of-the-art techniques such as tensor networks, but avoids introducing systematic errors due to truncation of the infinite-dimensional Hilbert space associated with superconducting phases. The approach is applied to fluxonium, a specific many-component superconducting qubit with favorable qualities for quantum computation. A systematic study of the influence of impedance on fluxonium is conducted that parallels previous experimental studies, and ground capacitance effects are explored. The qubit frequency and charge noise dephasing rate are extracted from statistical analyses of charge disorder, where thousands of instantiations of charge disorder in the Josephson junction array of a fixed fluxonium qubit are explicitly averaged over at the microscopic level. This is difficult to achieve with any other existing method.

115	**Multiqubit gate based on parity cross resonance**	Xuexin Xu	Contributed talk (17:00-17:15)

Xuexin Xu (1) Mohammad H. Ansari (1) Rihan Hai (2) Radhika Joshi (1) Siyu Wang (1)

(1) Forschungszentrum Jülich
(2) Delft University of Technology

The realization of multi-qubit entangling gates is essential for efficient, scalable, and fault-tolerant quantum information processing, reducing algorithmic complexity and circuit depth. We demonstrate a native three-qubit entangling gate implemented by simultaneously driving all qubits at a common frequency, exploiting engineered interactions to realize multi-control operations in a single coherent step. By optimizing the conditional dynamics originating from drive-induced nonlocal contamination, desired interaction channels are selectively enhanced while spurious terms are suppressed, ensuring robust performance within the computational subspace. This gate enables key
applications, including deterministic GHZ-state generation, Toffoli-class logic with a shortest gate duration of 90 ns and a highest fidelity of 99.72%, and a controlled-ZZ gate tailored for fast surface-code quantum error correction. Simulations based on realistic IBM device parameters indicate that the gate

maintains high fidelity and resilience under increasing excitation numbers and larger Hilbert-space dimensions. Our results establish a foundation for co-designing circuit architectures and control strategies that harness native multi-qubit interactions as fundamental building blocks for next-generation superconducting quantum processors, thereby enabling improved gate performance with more flexible tuning of circuit parameters.

97	**Polyfluxon: generalized fluxonium featuring *d*-degenerate fluxon states for qudit encoding**	Luca Chirolli	Contributed talk (17:15-17:30)

Luca Chirolli (1) Luigi Amico (2,3) Valentina Brosco (4) Gianluigi Catelani (5,6) Uri Vool (7)

(1) Department of Physics and Astronomy, University of Florence
(2) Technology Innovation Institute Abu Dhabi
(3) Department of Physics and Astronomy, University of Catania
(4) CNR-ISC
(5) Juelich Research Center
(6) Technology Innovation Institute
(7) Max Planck Institute for Chemical Physics of Solids

We propose a generalized fluxonium circuit hosting low-lying energy levels, well separated from the rest of the spectrum and that naturally realize a qudit system protected from leakage errors. The low-energy states are constituted by fractional fluxon states, localized in the minima of a suitably designed Josephson potential and weakly hybridized by quantum phase slip processes. The potential is tailored through a Fourier engineering approach, that employs multi-harmonics Josephson elements, which are in turn obtained from basic conventional elements by a proper scheme. We present the spectrum of a $d = 4$ and a $d = 5$ qudit system and then focus on the most relevant qutrit case. We analyze the dipole matrix elements for coupling to the radiation and we propose a non-Abelian, stimulate Raman adiabatic passage (STIRAP) protocol for single-qutrit gates, that is particularly suited for the present system. The proposed platforms opens novel perspectives in circuit engineering and quantum computing beyond the qubit paradigm.

659	**Quantum solitons and their quantum walks in transmon arrays**	Ben Blain	Contributed talk (17:30-17:45)

Ben Blain (1) Giampiero Marchegiani (1) Luigi Amico (1,2) Gianluigi Catelani (1,3)

(1) Quantum Research Center, Technology Innovation Institute, Abu Dhabi
(2) Department of Physics and Astronomy, University of Catania
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Superconducting qubits are artificial atoms whose spectra and interactions can be engineered through appropriate circuit design, a versatility that can be exploited for quantum simulation. We theoretically investigate a linear array of capacitively coupled transmons, effectively described by a Bose-Hubbard Hamiltonian with attractive interaction. We revisit the discrete-soliton nature of the lowest-energy band of the spectrum, and identify spatially localized quantum solitons. The solitonic character of these states is revealed through their dynamics, which displays a quantum interference pattern, or quantum walk, highlighting their composite nature. We discuss protocols for preparing spatially localized quantum solitons that are compatible with current state-of-the-art tunable-transmon circuits. Our results demonstrate that superconducting circuits provide a promising and experimentally accessible platform for the investigation of quantum soliton physics.

797	**Power-law suppression of superfluid stiffness in ultra-thin NbN films**	Meenakshi Sharma	Contributed talk (17:45-18:00)

Meenakshi Sharma (1)

(1) Max Planck Institute for Chemical Physics of Solids, Dresden

Ultrathin superconducting films have become the material of choice for compact, high-impedance microwave elements such as superinductors and kinetic-inductance detectors [1,2,4], because reduced dimensionality and disorder strongly enhance the kinetic inductance. Yet the same ingredients that boost it reshape the condensate itself: this property is set by the superfluid stiffness Θ, so enhancing one suppresses the other. This raises a question of both fundamental and technological significance—when disorder is used to engineer a large response, does it merely tune a circuit parameter, or fundamentally alter the condensate the device relies on? We address this directly using ultrathin NbN microwave resonators with thicknesses down to 2.8 nm [3], where the electrodynamic response grants simultaneous access to both the device-relevant inductance and the underlying superfluid stiffness.
Our thickness-controlled platform (25 nm → 2.8 nm) reaches a high sheet kinetic inductance near 300 pH/□, tuning disorder and dimensionality continuously within one technologically relevant material. We uncover an anomalous low-temperature power-law suppression of superfluid stiffness, incompatible with Mattis–Bardeen theory, that crosses over continuously into BCS-like electrodynamics as thickness increases [5]. We identify the governing parameter, Θ(0)/Tc, and show the characteristic energy scale obeys a two-scale relation, T0 ≈ 0.18 Θ(0) + 1.1 Tc, revealing that both phase stiffness and pairing gap set the electrodynamics, unlike the pure phase-stiffness limit reported near the SIT [5, 6]. NbN thus bridges the two regimes and serves as a practical quantum-circuit material: the kinetic inductance is intrinsic, while a self-terminating native oxide confines TLS loss to the extreme ultrathin limit.

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[2] V. Jouanny, S. Frasca, V. J. Weibel, L. Peyruchat, M. Scigliuzzo, F. Oppliger, F. De Palma, D. Sbroggiò, G. Beaulieu, O. Zilberberg, et al., Nat. Commun. 16, 3396 (2025).
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[6] A. V. Khvalyuk, T. Charpentier, N. Roch, B. Sacépé, and M. V. Feigel'man, Phys. Rev. B 109, 144501 (2024).

M10 – Session 3 (Tue 22, 10:30-12:30)			
ID	Title	Speaker	Type
232	**The Schmid transition in resistively shunted Josephson junction: BKT universality and transport properties**	Francesco Giuseppe Capone	Invited talk (10:30-11:00)

Francesco Giuseppe Capone (1) Antonio De Candia (1) Vittorio Cataudella (1) Rosario Fazio (2) Naoto Nagaosa Carmine Antonio Perroni (1) Giulio De Filippis (1)

(1) Dipartimento di Fisica "Ettore Pancini", Università degli Studi di Napoli Federico II - INFN, sezione di Napoli
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The Schmid transition represents a fundamental insulator-to-superconductor phase transition occurring in the resistively shunted Josephson junction (RSJJ). The system is modeled as a parallel circuit with a non-linear inductor (Josephson energy E_J), a capacitor (charging energy $E_C = 4e^2/2C$), and a shunt resistor R_S. Initially, Schmid and Bulgadaev [1,2] predicted this transition at $\alpha = R_q/R_S = 1$, with $R_q = h/4e^2$ being the resistance quantum. Nevertheless, recent theoretical [3,4] and experimental [5] studies have challenged its existence, reviving the debate on its transport implications. In this work, we clarify the transition's nature by introducing a distinct binary order parameter S. We establish that it falls into the Berezinskii-Kosterlitz-Thouless (BKT) universality class [6,7], evidenced by the logarithmic decay of correlation functions near the critical point. Employing linear response theory, we show the transition's hallmark is the weight of the delta function D_Q at $\omega = 0$ in the resistive response function $\Psi_{\mathrm{reg},Q}(\omega)$ [6]. Remarkably, it lacks a low-frequency Drude peak, demonstrating that dissipation is avoided even in the insulating phase. An out-of-equilibrium analysis under small injected currents further confirms this non-dissipative dynamics.

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383	**Kibble-Zurek Mechanism in the Open Quantum Rabi Model**	Tommaso Pirozzi	Contributed talk (11:00-11:15)

Tommaso Pirozzi (1) Grazia Di Bello (1) Vittorio Cataudella (1) Carmine Antonio Perroni (1) Giulio De Filippis (1)

(1) Università degli studi di Napoli Federico II

The non-equilibrium response of many-body quantum systems to time-dependent driving remains a central frontier in modern physics, with profound implications for quantum simulator architectures such as superconducting circuits. A primary challenge in these platforms is the preparation of highly correlated states through quantum phase transitions (QPTs), where the unavoidable critical slowing down forces a breakdown of the adiabatic regime. The Kibble-Zurek mechanism (KZM) provides a cornerstone framework for predicting defect formation in such dynamics. While Markovian dissipation typically compromises universal scaling due to the competition between extrinsic noise, internal relaxation, and quench dynamics, the impact of non-Markovian memory remains largely unexplored.
In this work, we investigate the validity of the KZM in the Open Quantum Rabi Model (OQRM) coupled to a non-Markovian Ohmic bath. Notably, this model has been simulated in the deep strong coupling regime using a quantum circuit with flux qubits. The dynamics is governed by the Hamiltonian $H = H_{\text{Q-O}} + H_I$, with $H_{\text{Q-O}} = -\frac{\Delta}{2}\sigma_x + \omega_0 a^\dagger a + g\sigma_z(a^\dagger + a)$. The term $H_I = \sum_i \left[\frac{p_i^2}{2M_i} + \frac{k_i(x-x_i)^2}{2}\right]$ accounts for a bath of harmonic oscillators coupled to the resonator coordinate $x = \sqrt{1/2m\omega_0}(a + a^\dagger)$.
Using advanced Matrix Product State simulations (DMRG and TDVP), we demonstrate that environmental memory induces a Berezinskii-Kosterlitz-Thouless (BKT) transition. This criticality is dynamically witnessed by the equilibrium relaxation time τ, which follows the scaling behavior $\tau(g) \propto \exp\left(\frac{B}{\sqrt{|g-g_c|}}\right)$. By implementing linear quenches across the critical point, we show that the excitation energy E_{exc} evaluated at the exact freeze-out time t_f reveals a robust universal power-law scaling $E_{\text{exc}} \propto t_f^{-\mu}$.
Crucially, since the non-Markovian bath redefines the underlying universality class, dissipation does not inherently compete with adiabatic dynamics. The non-equilibrium response is accurately captured by a renormalized two-level framework, establishing the KZM as a reliable probe of criticality in open quantum systems.

67	**Photon counting beyond the rotating-wave approximation**	Steven Kim	Contributed talk (11:15-11:30)

Steven Kim (1) Fabian Hassler (1)

(1) RWTH Aachen

Open quantum systems are often described by a Lindblad master equation, which relies on a set of approximations, most importantly the rotating-wave approximation which is only valid for weak damping. In the Lindblad setting, dissipative processes are described through jump operators, distinguishing between absorption and emission of photons. This enables the simple identification of emitted photons which provides a straightforward way to obtain the radiation statistics. Outside the rotating-wave limit, the Lindblad approach does not work. Open quantum systems can then be described by, e.g., the quantum Langevin equation. However, in this framework the number of emitted photons is not easily accessible. In this work, we point out how to obtain the photon counting statistics from a quantum Langevin equation and provide an expression for the photon current operator, for arbitrary systems coupled to

linear environments. As an example, we employ the method to study the radiation statistics of a damped harmonic oscillator at finite temperature beyond the rotating-wave approximation. We show that even outside the rotating-wave limit, the most important contribution to the radiation statistics can be captured by an effective Lindblad equation, thus extending the range of possible applications of the Lindblad framework.

445	**Thermodynamic uncertainty relations for superconducting hybrid systems**	Fabio Taddei	Contributed talk (11:30-11:45)

Fabio Taddei (1) Rosario Fazio (2) Michele Governale (3) Franco Mayo (4) Nahual Sobrino (2)

(1) NEST, Istituto Nanoscienze-CNR
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(3) Victoria University of Wellington, New Zealand
(4) Universidad de Buenos Aires, Argentina

Stability–efficiency trade-offs in nonequilibrium transport are constrained by thermodynamic uncertainty relations (TURs), which bound current fluctuations in terms of entropy production. In hybrid normal–superconducting (N–S) devices, however, the status of quantum TURs has remained unclear. Here we investigate Andreev-mediated transport and fluctuations in N–S junctions and quantum-dot systems, including the effects of superconducting coherence and Coulomb interactions. In the subgap (Andreev) regime, we show that deviations from the normal quantum TUR are governed by macroscopic superconducting coherence quantified by the pair amplitude, while dephasing or interactions suppress this coherence and restore conventional bounds. We derive a hybrid quantum TUR valid for all two-terminal N–S junctions in the Andreev regime, which is never violated, is saturated only at vanishing current, and connects to the normal quantum bound via the substitution e —> 2e. Using real-time diagrammatics and full counting statistics, we compute current, noise, and entropy production for interacting N–S quantum dots in the large-gap limit. Coulomb interactions renormalize resonant transport and strongly reduce current precision, especially at high temperatures where average currents are weakly affected. Our results establish a direct link between superconducting coherence, interactions, and nonequilibrium fluctuations, and identify current precision as a robust probe of interacting Andreev transport.

329	**Systematic studies on high *Q*i tantalum resonators**	Francesca D'Esposito	Contributed talk (11:45-12:00)

Wael Ardati (1) Olivier Buisson (2) Giulio Cappelli (1) Thierry Crozes (1) Ivana Curci (3) Francesca D'Esposito (1) Bruno Fernandez (1) Quentin Ficheux (2) Weibke Hash-Guichard (1) Yasmine Kalboussi Shelender Kumar (1) Simon Le Denmat (1) Cyril Mori (1) Eric Mossang (1) Cecile Naud (1) Dorian Nicolas (1) Thomas Proslier (3) Julien Renard (1) Nicolas Roch (2) Francisco Rouxinol (4) Lucas Ruela (1) Vishnu Suresh (1) Jean-Samuel Tettekpoe (1)

(1) NEEL INSTITUT CNRS
(2) Institut NEEL-CNRS-UGA
(3) Université Paris-Saclay-CEA
(4) State University of Campinas

Superconducting qubit performance is fundamentally limited by decoherence mechanisms, notably dielectric losses. In this work, we investigate a transmon molecule design featuring an original coupling mechanism that enables a non-perturbative cross-Kerr interaction between the qubit and the readout microwave cavity [1]. This architecture has already demonstrated high readout fidelity (99.2% [2]) along with long coherence times ($T_1 \simeq 120$ µs and $T_2 \simeq 23$ µs [2]). Our objective is to implement such a transmon molecule using tantalum capacitive pads in conjunction with aluminum Josephson junctions. Recent advances indicate that tantalum (Ta) deposited on sapphire substrates can significantly enhance qubit performance, with relaxation times (T_1) reaching the millisecond range [3].
The tantalum thin films are grown on sapphire substrates by electron-beam evaporation in an ultra-high-vacuum chamber with a base pressure of approximately 5×10^{-10} mbar. To investigate the influence of growth conditions on superconducting and microwave properties, films are deposited at different substrate temperatures, including 350 °C and 580 °C.
We characterize the structural, morphological, and superconducting properties of the films using X-ray diffraction, atomic force microscopy (AFM), and resistance-versus-temperature measurements. To evaluate microwave losses, we fabricate coplanar waveguide resonators and measure their internal quality factors. We obtain values ranging from 6×10^6 in the low-photon-number regime to above 6×10^7 at high microwave drive power, placing our devices among state-of-the-art superconducting resonators. Finally, we perform systematic measurements of the internal quality factor and resonance frequency as functions of temperature and microwave drive power. The data are analyzed within the frameworks of two-level systems (TLS), Mattis–Bardeen theory, and Ginzburg–Landau theory to account for dielectric losses, quasiparticle contributions, and nonlinear behavior. Interestingly, from these measurements, we observe significant spatial variations of the superconducting critical temperature () across devices fabricated on the same wafer. These spatial variations depend on the substrate temperature during evaporation. They have been observed in several recent studies and their origins are still in debate [4]. By local probe using point contact tunnelling spectroscopy, we were able to relate them to superconducting gap variations.

[1] R. Dassonneville et al, Phys. Rev. X 10, 011045 (2020).
[2] C. Mori, V. Milchakov, et al., High-power readout of a transmon qubit using a nonlinear coupling, arXiv:2507.03642 (2025).
[3] A. Place et al. Nature communications 12.1 (2021).
[4] F. Bahrami et al. Phys. Rev. B 113, 054505 (2026).

518	**Granular aluminum superinductors**	Thomas Reisinger	Contributed talk (12:00-12:15)

Lucas Brauch (1) Simone Dehm (1) Nicolas Gosling (1) Mahya Khorramshahi (1) Ralph Krupke (1,2) Christian Kübel (1,2) Patrick Paluch (1) Ioan Pop (1,3) Thomas Reisinger (1) Martin Spiecker (1) Wolfgang Wernsdorfer (1) Nicolas Zapata (1)

(1) Karlsruhe Institute of Technology
(2) Technical University of Darmstadt
(3) University of Stuttgart

Superconducting circuits are a promising platform for fault-tolerant quantum computing, quantum-limited amplification, ultra-low-power electronics, and sensors with ultimate sensitivity. Reducing loss and fabrication complexity in these circuits is therefore of significant interest.
Superinductors — superconducting inductors with impedances exceeding the resistance quantum — enable the development of protected qubits and enhance coupling to systems with small electric dipole moments. While Josephson-junction chains are a common approach, superinductors can also be realized using traces of disordered nanocomposite superconductors, such as granular aluminum (grAl). We explore the limits of impedance in grAl ring resonators, demonstrating inductances up to 4 µH and impedances exceeding 100 kΩ in the technologically relevant 4–8 GHz range. Despite these high

impedances, the resonators maintain quality factors on the order of 10^5, making them well-suited for quantum information processing. Notably, they are fabricated in a single-step, zero-angle e-beam lift-off lithography process.

519	**On the intrinsic nonlinearity of granular aluminium**	Mitchell Field	Contributed talk (12:15-12:30)

Mitchell Field (1) Ioan M. Pop (1) Nicolas Zapata (2)

(1) Karlsruhe Institute of Technology (IQMT)
(2) Qilimanjaro Quantum Tech

Over the last 10 years, granular aluminium has risen as a popular material for implementation in superconducting circuits thanks to its high kinetic inductance, low loss with approachable fabrication.
Where granular aluminium really shines is as the nonlinear element for parametric amplification, showing both magnetic field resilience, robustness for multi pumping schemes with a compact footprint. In this talk we compare grAl to other disordered superconductors and junction arrays and show how its tuneable nonlinearity stands out.

M10 – Session 4 (Tue22, 16:00-18:00)

ID	Title	Speaker	Type
310	**Doppler-induced tunable and shape-preserving frequency conversion of microwave wave packets**	Gianluca Rastelli	Contributed talk (16:00-16:15)

Felix Ahrens (1) Enrico Bogoni (1) Iacopo Carusotto (2,3) Nicolò Crescini (1) Andrea Giachero (4) Alessandro Irace (1) Federica Mantegazzini (1) Renato Mezzena (3) Gianluca Rastelli (2,3) Andrea Vinante (5)

(1) Fondazione Bruno Kessler (FBK), Trento, 38123, Italy.
(2) Pitaevskii BEC Center, CNR-INO
(3) Dipartimento di Fisica, Università di Trento
(4) Department of Physics, University of Milano-Bicocca
(5) CNR-IFN

The rapid advancement of quantum electronics and microwave photonics is driven by the native operation of superconducting qubits, spin qubits, and hybrid solid-state quantum devices in the microwave regime. This makes microwave photonics a powerful platform for their precise control and manipulation, while superconducting-circuit-based quantum microwave photonics opens new avenues for engineering photonic states.
We introduce and experimentally demonstrate a Doppler-induced frequency conversion technique for microwave pulses at cryogenic temperatures. The method is intrinsically free from intermodulation and pulse-shape distortions, while offering high tunability. It relies on the spatiotemporal modulation of an effective refractive medium, enabling efficient and controllable frequency translation.
The implementation is based on a superconducting high-kinetic-inductance transmission line, where a microwave pulse counter-propagates with a control current front [1]. In this travelling-wave configuration, we achieve frequency shifts of microwave wave packets at 500 MHz and 4 GHz of up to 3.7%, with full preservation of their temporal profiles.

[1] https://arxiv.org/abs/2603.12436

342	**A topological Josephson parametric amplifier array: Directional, broadband, and low-noise amplification**	Tomas Ramos	Contributed talk (16:15-16:30)

Tomas Ramos (1) Juan Jose Garcia-Ripoll (1) Alvaro Gomez-Leon (1) Alejandro Gonzalez-Tudela (1) Diego Porras (1) Dian Tan (2) Jingchao Zhao (2)

(1) IFF-CSIC Madrid
(2) Southern University of Science and Technology, Shenzhen

Directional amplification is a critical requirement for scalable superconducting quantum computing, yet current solutions rely on bulky, off-chip ferrite isolators that hinder integration. Here we propose a fully on-chip, directional and broadband superconducting quantum amplifier whose isolation arises intrinsically from topological properties. The setup consists of a Josephson junction array (JJA) weakly coupled to an auxiliary array of linear resonators with impedance matching conditions on its boundaries. A strong pump injected at one end of the auxiliary array propagates unidirectionally without reflections, inducing an effective pump on the JJA that simultaneously provides phase matching and activates four-wave mixing processes. The propagation phase of this pump breaks time-reversal symmetry, rendering parametric amplification intrinsically directional with backscattering exponentially suppressed — a direct manifestation of the non-trivial topology induced in the JJA. Stability is achieved by engineering local losses on all JJA sites, which can be realized either by coupling each site to an external transmission line or by incorporating on-chip resistor elements, allowing the system to dissipate excess energy from the pump.
We fully characterize the directional amplifying properties of the device through approximate quantum input-output simulations and exact semi-classical SPICE simulations. For state-of-the-art parameters, a compact device with N~10 sites achieves gains above 20 dB, bandwidths of hundreds of MHz, and reverse isolation beyond -30 dB, while operating near the quantum noise limit. Topological protection provides robustness against fabrication disorder, reducing gain ripples, and power saturation can be mitigated by diluting each JJA non-linearity into a small sub-array of M~3 Josephson junctions in series. This work establishes an alternative route toward fully on-chip quantum microwave amplifiers.

358	**Frequency-space analogy in a superconducting microwave cavity: Bloch-wave dynamics in a synthetic lattice and truncated SU(1,1) interferometry**	Alessandro Irace	Contributed talk (16:30-16:45)

Alessandro Irace (1,2) Felix Ahrens (1) Enrico Bogoni (1,2) Giulio Cappelli (1) Iacopo Carusotto (3,4,5) Nicolò Crescini (1) Marcello Faggionato (1,2) Paolo Falferi (1) Andrea Giachero (2,6) Federica Mantegazzini (1) Benno Margesin (1) Renato Mezzena (5,7) Gianluca Rastelli (3,4,5) Andrea Vinante (8)

(1) Fondazione Bruno Kessler, (2) Università Bicocca, (3) Pitaevskii BEC Center, (4) CNR-INO, (5) Univeristy of Trento, (6) INFN Milano Bicocca, (7) INFN-TIFPA, (8) IFN-CNR

Superconducting microwave circuits provide a versatile platform for exploring both fundamental topological physics and the frontiers of quantum metrology. In this talk, we present two advancements based on the coherent manipulation of frequency modes in planar tunable resonators. First, we demonstrate how frequency-based synthetic dimensions can expand the dimensionality of photonic systems. By periodically modulating a single-mode resonator under a coherent monochromatic drive, we realize a tilted synthetic lattice. We study the resulting Bloch wave dynamics and their unique spectral signatures, providing experimental confirmation via a tunable superconducting resonator. Second, we exploit parametric processes to surpass the standard quantum limit in interferometry. We present a microwave device based on a single flux tunable Josephson Parametric Amplifier operating as a truncated SU(1,1) interferometer. In our implementation, the two distinct frequencies of the signal and idler photons act as the two arms of the interferometer, allowing them to travel along the same physical waveguide. By employing digital demodulation, we achieve a setup capable of reaching the Heisenberg scaling limit with minimal hardware overhead.

548	**On calorymetric detection of microwave photons via proximity effect**	Michal Horodecki	Contributed talk (16:45-17:00)

Jukka Pekola (1) Marcin Lobejko (2) Paulina Janowicz (2) Peter Samuelsson (3) Andrzej Grudka (4) Michal Horodecki (2)

(1) Aalto University
(2) ICTQT University of Gdańsk
(3) Lund University
(4) Adam Mickiewicz University Poznań

One of the challenges of mesoscopic physics is calorimetric detection of microwave photons. It requires samples of ultrasmall heat capacity of order of Boltzmann constant. Here we investigate possibility of using proximitized metal for this purpose. First, we point out that the small heat capacity implies also small absorption rate. We show a trade-off between quantum efficiency of calorimetric detection and signal-to-noise ratio. The trade-off is demonstrated for mini-gap developed in proximitized metal, and the mini-gap is analysed both in terms of simple model as well as by means of Usadel equation. As a result we can obtain decent efficiency and reasonable signal-to-noise ration at the same time. Finally, the mini-gap may result in two electron temperatures (above and below mini-gap) due to small equilibration rate across the mini-gap. We propose a procedure of calibration of the thermometer in such circumstances.

429	**Quartet correlations revealed in the noise signatures of superconducting nanodevices**	Jordi Picó Cortés	Contributed talk (17:00-17:15)

Jordi Picó Cortés (1) Luca Chirolli (1)

(1) Università degli Studi di Firenze

Cooper quartets are an exotic electronic state composed of correlated four electron excitations, generalizing the concept of Cooper pairs to charge-4e superconductors. While the latter are yet to be realised experimentally as a macroscopic phase, hybrid superconducting nanodevices may offer a highly-tunable and well-studied platform for the realisation and investigation of quartet states. Following [1], we study signatures of Cooper quartets in a system composed of a double quantum dot (DQD) coupled to normal and superconducting leads in the limit of large gap. In this configuration, we show non-equilibrium signatures of quartet correlations in the current noise, allowing the experimental detection of quartet states in a controllable, well-understood setting.

[1] L. Chirolli, A. Braggio, and F. Giazotto, Phys. Rev. Res. 6, 033171 (2024).

455	**Artificial topological insulator realized in a two-terminal Josephson junction with Rashba spin-orbit interaction**	Tomaž Rejec	Contributed talk (17:15-17:30)

Luka Medic (1) Tomaž Rejec (1) Anton Ramšak (1)

(1) Faculty of mathematics and physics, University of Ljubljana

We study a two-terminal Josephson junction with conventional superconductors and a normal region with Rashba spin-orbit interaction, characterized by two Aharonov-Casher (AC) fluxes. When the superconducting phase difference equals π, the Andreev subgap spectrum may host zero-energy Weyl singularities associated with a vanishing normal-state reflection eigenvalue. With one of the AC fluxes playing the role of a quasimomentum, the junction can be viewed as an artificial one-dimensional chiral topological insulator. Its topological phase can be tuned by crossing a Weyl singularity by means of varying the remaining AC flux. By associating an additional component of the quasimomentum with the superconducting phase difference, an artificial Chern insulator is realized.

263	**Switching-Current Signatures of Magnetic Avalanches in InAs/Al Nanowire Josephson Junctions**	Claudio Guarcello	Contributed talk (17:30-17:45)

Claudio Guarcello (1) Ofelia Durante (1) Roberta Citro (1) Elia Strambini (2) Valeria Demontis (3) Mirco Rocci (4) Alessandro Braggio (2) Sergio Battiato (5) Valentina Zannier (2) Lucia Sorba (2) Francesco Giazotto (2)

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We report switching-current signatures of magnetic avalanches in an -doped InAs/Al nanowire Josephson junction. Under a perpendicular magnetic field, the device exhibits a low-field Fraunhofer-like modulation of the switching current together with reproducible discrete jumps appearing at $|B| \approx 3$ mT. These features separate distinct switching-current branches and show a clear sweep-history dependence.
By tracking the relevant field scales from 30 to 900 mK, we find that the jump field remains nearly temperature independent, in sharp contrast with the superconducting critical field, which follows the expected thermal suppression of Al. This distinction rules out conventional superconductivity-suppression mechanisms as the primary origin of the observed switching and instead points to a magnetically active subsystem coupled to the weak link.
We interpret the data in terms of avalanche-like reconfigurations of a metastable magnetic texture in the hybrid nanowire environment. Within an effective-field picture, each reconfiguration generates a discrete local-field offset that modifies the Josephson response and converts magnetic switching into abrupt transport discontinuities.
Our results identify hybrid nanowire Josephson junctions as sensitive probes of intrinsic magnetic dynamics at low magnetic fields and highlight their potential as mesoscopic hybrid platforms where superconducting transport directly reveals emergent magnetic degrees of freedom.

See arXiv:2603.29757 (2026)

517	**Impact of anisotropic Polar and Anderson-Brinkman-Morel phases of p-wave superconductors on thermoelectrics properties of quantum dot based hybrid**	Vrishali Sonar	Contributed talk (17:45-18:00)

Vrishali Sonar (1) Piotr Trocha (1)

(1) Institute of Spintronics and Quantum Information, Faculty of Physics, Adam Mickiewicz University

P-wave superconductors [1] host rich quantum phenomena arising from odd-parity, anisotropic, spin-triplet pairing, including nontrivial topology, Majorana physics, and time-reversal symmetry breaking. In particular, chiral and anisotropic p-wave phases strongly influence quasiparticle transport and Andreev reflection, offering promising routes for superconducting spintronics. However, theoretical/computational studies of Quantum dot (a mesoscopic scatterer) based hybrid systems incorporating p-wave superconductors remain comparatively underexplored [2][3].
We theoretically study thermoelectric transport in a hybrid device consisting of a quantum dot coupled to a ferromagnetic lead and a spin-triplet p-wave superconductor. Focusing on the Polar and Anderson-Brinkman-Morel (ABM) phases, we incorporate momentum-dependent tunneling via an angle-dependent coupling modelling and analyze configurations where the superconducting symmetry axis is parallel or perpendicular to the tunneling direction. Using Keldysh Green's function formalism in the linear-response regime, we compute electrical and thermal conductances, thermopower, and the thermoelectric figure of merit.
Our results demonstrate that gap anisotropy and orientation play a decisive role in transport, producing strong phase- and geometry-dependent signatures. In particular, anisotropy governs the balance between Andreev reflection and quasiparticle tunneling, allowing the effective triplet Andreev reflection to be suppressed or enhanced by rotating the superconducting axis. In the ABM phase, this behavior is traced to the azimuthal phase structure of the order parameter. Additionally, thermal conductance is enhanced by orders of magnitude compared to the s-wave case[4]. These findings establish thermoelectric transport as a sensitive probe of triplet pairing symmetry and nodal structure in p-wave superconductors.
We note that the approach can be extended for non-equilibrium studies and any superconducting states for which the gap function angular dependence is predicted. These results may assist experimental efforts.

M10 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
522 **P010**	**On demand emission of the electron-hole superposition from a proximitized quantum dot**	Krzysztof Pyrchla	Poster

Andrzej Grudka (1) Michał Horodecki (2) Ankit Kumar (3) Mykhailo Moskalets (4,5) Krzysztof Pyrchla (6) Kyrylo Snizhko (7)

(1) Adam Mickiewicz University in Poznań
(2) International Centre for Theory of Quantum Technologies
(3) Technion - Israel Institute of Technology
(4) Institute for Cross-Disciplinary Physics and Complex Systems IFISC (UIB-CSIC)
(5) Department of Metal and Semiconductor Physics, NTU "Kharkiv Polytechnic Institute"
(6) Faculty of Electronics, Telecommunications and Informatics, Gdansk University of Technology
(7) CEA Grenoble

We investigate the interplay between on-demand single-electron emission and superconducting correlations within the framework of electron quantum optics. Specifically, we study a semiconductor quantum dot proximitized by a superconductor and driven by a time-dependent electrostatic potential.
In the absence of superconductivity, a driven quantum dot may operate as a single-electron emitter, generating clean, quantized electron wave packets on demand, as demonstrated in Ref. [1]. In this regime, raising the dot energy level above the Fermi energy results in a deterministic emission of an electron into the lead.
Here, we explore how this emission mechanism is fundamentally modified when superconducting proximity effects are present. Due to induced pairing, the quantum dot no longer hosts states with a well-defined particle number, but instead supports coherent superpositions of empty and doubly occupied states. As a consequence, driving the dot does not simply lead to electron emission. Instead, two competing processes emerge: (i) emission of an electron to the lead and (ii) hole emission to the lead due to Andreev reflection.
We show that this mechanism enables the controlled generation of coherent electron–hole superpositions. Importantly, these are superpositions of an electron and a hole, not electron-hole pairs. We analyze the emission process and the properties of the resulting superposition.

[1] J. Keeling, A. V. Shytov, and L. S. Levitov, "Coherent Particle Transfer in an On-Demand Single-Electron Source," Phys. Rev. Lett., vol. 101, no. 19, p. 196404, Nov. 2008, doi: 10.1103/PhysRevLett.101.196404.

816 **P011**	**Modeling Superconducting Circuits with Neural Stochastic**	Lukas Sotak	Poster

Lukáš Soták (1) Artem Ryabov (2) Tomáš Novotný (1) Martin Žonda (1)

(1) Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Ke Karlovu 5, Praha 2 CZ-121 16, Czech Republic
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uperconducting circuits containing Josephson junctions are important for both fundamental research and applications ranging from precision metrology to quantum technologies. Even relatively simple circuits exhibit rich nonlinear dynamics, including phase slips and switching between different dynamical regimes [1]. Such systems are often well described by the resistively and capacitively shunted junction (RCSJ) model and its extensions. However, reliable models of more complex and noisy circuits are often difficult to formulate. In this work, we employ neural stochastic differential equations [2], a machine-learning approach that combines known physical models with neural networks to describe such systems. The neural network learns the missing contributions to the dynamics, including stochastic effects, while preserving consistency with the underlying physics. The approach is sufficiently flexible to describe different circuit architectures and may provide a general framework for modeling complex superconducting circuits. As a proof of concept, we apply the method to RCSJ models with different Josephson potentials [3,4] and a more complex circuit.

[1] M. Žonda, W. Belzig, T. Novotný, Phys. Rev. B 91 (13), 134305 (2015)
[2] X. Li, T.-K. L. Wong, R. T. Q. Chen, D. Duvenaud, Proc. Mach. Learn. Res. 108, 3870-3882 (2020)
[3] M. Žonda, W. Belzig, E. Goldobin, T. Novotný, Phys. Rev. B 110 (5), 054306 (2024)
[4] F. Dominguez, F. Hassler, G. Platero, Phys. Rev. B 86, 140503(R) (2012)

M11 - Electron-Phonon Coupling in Correlated Quantum Matter

M11 – Session 1 (Mon 21, 10:30-12:30, Chair: Thomas Schaefer)			
ID	Title	Speaker	Type
98	**Impact of Spin–Phonon Interactions on Magnetism in Frustrated Triangular and Kagome Lattices**	Roser Valenti	Invited talk (10:30-11:00)

Roser Valenti (1)

(1) Goethe University Frankfurt

The nature of the ground state of the spin-1/2 Heisenberg model on frustrated triangular and kagome lattices remains a central question in quantum magnetism. Here, we will present a variational Monte Carlo study of a spin–phonon Hamiltonian on the triangular and kagome lattices, fully incorporating quantum dynamics of both spins and phonons., and will discuss possible instabilities of the underlying quantum spin liquid groundstate towards the presence of a spin-phonon interaction [1-2]. We will discuss the implications of the results on quantum materials.

[1] Ferrari et al. Phys. Rev. B 109, 165133 (2024)
[2] Ferrari et al. Phys. Rev. Research 7, L042053 (2025)

This work has been done in collaboration with Francesco Ferrari, Josef Willsher, Urban F. P. Seifert, Johannes Knolle and Federico Becca

731	**Electron-Phonon Interaction and Strong Correlations: Friends or Enemies?**	Massimo Capone	Invited talk (11:00-11:30)

Massimo Capone (1)

(1) SISSA - International School for Advanced Studies - Trieste

A widespread belief treats electron–phonon and electron–electron (Hubbard) interactions as mutually exclusive, assuming a direct competition in which one interaction dominates while the other becomes irrelevant.
In this talk, I will discuss how this scenario—although justified in some materials—is challenged in many modern quantum systems, ranging from alkali-metal-doped fullerides [1] to magic-angle twisted bilayer graphene [2]. To shed light on this interplay, I will start from simplified models, comparing and contrasting the widely studied single-band Hubbard–Holstein model [3] with multi-orbital models featuring different types of phonon couplings. The main result is that phonon modes coupled to the local charge tend to compete with Hubbard repulsion, whereas other modes—such as Jahn–Teller phonons—can coexist with electronic correlations, leading to a rich interplay with Hund's exchange interaction. As a consequence, qualitatively different physical scenarios emerge: in some cases, strongly correlated phases are largely unaffected by phonons, while in others phononic effects are enhanced. This can give rise, for instance, to phases where Mott physics coexists with bipolaronic features [4], or to correlation-enhanced phonon-mediated superconductivity [1]. Finally, I will discuss how these scenarios manifest in different classes of materials with diverse properties, including superconductors (such as fullerides and magic-angle twisted bilayer graphene) and excitonic insulators.

[1] M. Capone, M. Fabrizio, C. Castellani, and E. Tosatti, Rev. Mod. Phys. 81, 943 (2009); Y. Nomura et al. Science Advances 1, e1500568 (2015).
[2] M. S. Liang et al., arXiv:2604.04631
[3] M. Capone, C. Castellani, and M. Grilli, Adv. Cond. Mat. Phys. 2010, 920860 (2010)
[4] A. Scazzola, A. Amaricci and M. Capone, Phys. Rev. B 107, 085131 (2023)
[5] S. Giuli et al. 2026

This work is based on collaborations with several researchers, including the authors of the cited studies.

116	**Nonperturbative interplay of charge and spin fluctuations in the Hubbard-Holstein model**	Emin Moghadas	Contributed talk (11:30-11:45)

Emin Moghadas (1) Alessandro Toschi (1) Andrew Millis (2)

(1) Institute of Solid State Physics, TU Wien
(2) Columbia University

We present a dynamical mean-field study of the Hubbard–Holstein model in the strong-coupling regime. We demonstrate that the interplay between local spin and charge fluctuations, driven by strong electron–electron and electron–phonon interactions, stabilizes commensurate charge-density-wave order over a broad range of electron densities. Remarkably, this phase persists even at fillings that are incompatible with conventional checkerboard charge order. By analyzing the symmetry-broken phase, we gain further insight into the thermodynamic properties and energetics of this state. Using inhomogeneous dynamical mean-field theory, we identify the physical mechanism responsible for stabilizing the charge-ordered regime.

473	**Intertwined fluctuations and Isotope effects in the Hubbard-Holstein model from functional renormalization**	Aiman Al-Eryani	Contributed talk (11:45-12:00)

Aiman Al-Eryani (1) Sabine Andergassen (2) Michael Scherer (1)

(1) Ruhr Uni Bochum
(2) TU Wien

Electron-electron and electron-phonon interactions are responsible for the formation of spin, charge, and superconducting correlations in layered quantum materials. A paradigmatic model for such materials that captures both kinds of interactions is the two-dimensional Hubbard-Holstein model with a dispersionless Einstein phonon.

In this work, we provide a detailed analysis of the magnetic, density, and superconducting fluctuations at and away from half-filling. To that end, we employ the functional renormalization group using the recently introduced extension of the single-boson exchange formulation. More precisely, we go beyond previous approaches to the model by resolving the full frequency dependence of the two-particle vertex and taking into account the feed-back from the electronic self-energy. We perform broad parameter scans in the space of Hubbard repulsion, electron-phonon coupling strength, and phonon frequency to explore the leading magnetic, density, and superconducting susceptibilities from the adiabatic to the anti-adiabatic regime.
Our numerical data reveal that self-energy effects lead to an enhancement of the d-wave superconducting susceptibility towards larger phonon frequencies, in contrast to earlier isotope-effect studies. At small phonon frequencies, large density contributions to the s-wave superconducting susceptibility change sign and eventually lead to a reduction of s-wave superconductivity with increasing electron-phonon coupling, signaling the breakdown of Migdal-Eliashberg theory. We analyze our findings systematically, employing detailed diagnostics of the intertwined fluctuations and pinning down the various positive and negative isotope effects of the physical susceptibilities.

529	**Exchange striction controls demagnetization in antiferromagnetic insulators**	Ravi Kaushik	Contributed talk (12:00-12:15)

Ravi Kaushik (1) Sergey Artyukhin (2) Aleksandr Buzdakov (1) Alexei Kimel (3)

(1) Italian Institute of Technology
(2) Quantum Materials Theory, Genova, Italy
(3) Radboud University

Ultrafast order melting in magnetic insulators is governed by two processes: intrinsic intra-spin relaxation and spin-lattice energy transfer. Antiferromagnets, which lack net magnetization, can in principle evade angular-momentum constraints and display markedly faster order-parameter dynamics than ferromagnets, but experimental rates vary widely across materials. Here we combine first-principles magnetostriction calculations, phonon and magnon spectral analysis, atomistic spin-dynamics simulations and time-resolved second-harmonic generation to disentangle these pathways and explain material-dependent disparities. Focusing on two structurally similar antiferromagnets, Cr2O3 and FeBO3, we show that the strength of spin-phonon coupling - revealed by magnetostrictive response and phonon-magnon spectral overlap - dictates the dramatic difference in order-melting rates. We also achieved accelerated dynamics in Cr2O3 and show sub-2-ps order melting in both experiment and simulation. Our results establish spin-phonon coupling as the decisive control parameter for ultrafast antiferromagnetic dynamics and provide a practical framework to design faster switching in antiferromagnetic spintronic devices.

146	**Relevance of Lattice Disorder, Correlations, and Oxygen Dopants on Iron under Earth Core Conditions**	Markus Aichhorn	Contributed talk (12:15-12:30)

Markus Aichhorn (1) Dario Alfe (2) German Blesio (3,4) Jernej Mravlje (5) Leonid Pourovskii (6) Monica Pozzo (7)

(1) Graz University of Technology
(2) Department of Earth Sciences and London Centre for Nanotechnology, University College London, Gower Street, London, WC1E 6BT, UK
(3) Instituto de Física Rosario (CONICET)
(4) Facultad de Ciencias Exactas, Ingeniería y Agri- mensura, Universidad Nacional de Rosario, Rosario, Santa Fe, 2000, Argentina
(5) Jožef Stefan Institute, Jamova 39, Ljubljana, SI-1000, Slovenia
(6) CPHT, CNRS, Ecole polytechnique, IP Paris, 91120 Palaiseau France
(7) Faculty of Technological & Innovation Sciences, Universitas Mercatorum, Piazza Mattei 10, Rome, 00186, Italy

Knowing the transport properties of iron under realistic conditions present in the Earth's core is essential for the geophysical modeling of Earth's magnetic field generation. In addition to the effects of extreme pressures and temperatures, which cause dominant scattering due to thermal disorder, transport can also be affected by light elements and electron-electron interactions. Using a combination of molecular dynamics, density functional theory, and dynamical mean-field theory, we studied the impact of oxygen impurities on electronic correlations and their joint effect on transport in Earth's liquid outer core. Our findings reveal that oxygen inclusion moderately enhances electronic correlations. Both oxygen impurities and increased electronic correlations reduce thermal conductivity by ~20% each, hence playing an equally critical role in stabilizing the geodynamo.

M11 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
69 **P012**	**Unbiased functional renormalization group study of Su-Schrieffer-Heeger phonons in the two-dimensional Hubbard model**	Francesco Domizio	Poster

Francesco Domizio (1) Aiman Al-Eryani (2) Sabine Andergassen (1) Michael M. Scherer (2)

(1) Institute of Information Systems Engineering and Institute of Solid State Physics, Vienna University of Technology, 1040 Vienna, Austria
(2) Theoretical Physics III, Ruhr-University Bochum, 44801 Bochum, Germany

We study the two-dimensional Hubbard model coupled to Su–Schrieffer–Heeger phonons on the square lattice using a recently developed generalization of the single-boson exchange formalism for extended interactions. The functional renormalization group description retains the full frequency dependence of the two-particle vertex and the electronic self-energy and allows for an unbiased analysis of magnetic, charge, and superconducting fluctuations. We perform extensive parameter scans in terms of the Hubbard interaction, the electron–phonon coupling strength, and the phonon frequency, ranging from the adiabatic to the antiadiabatic regime. In the absence of the Hubbard interaction, we find that the threefold degeneracy of antiferromagnetic order, charge-density-wave order, and s-wave superconductivity at half filling holds for all phonon frequencies. In the adiabatic limit, however, the leading instability is a valence bond solid state. For finite values of the Hubbard interaction, the $\mathbb{Z}_{2,\text{Shiba}}$ symmetry is lifted, leading to a competition between antiferromagnetism

and valence bond order. Finally, at finite doping, the interplay between the Hubbard interaction and the Su–Schrieffer–Heeger phonons leads to an even richer picture characterized by intertwined ordering tendencies.

357 **P013**	**Spin-Phonon Coupling in Tetragonal Europium Titanate: First-Principles Insights into Magnetic Field-Induced Dielectric Shifts**	Archit Banerjee	Poster

Venimadhav Adyam (1) Archit Banerjee (1)

(1) Cryogenic Engineering Centre, IIT Kharagpur

The quantum paraelectric perovskite $EuTiO_3$ exhibits anomalous cross-coupling between its magnetic ordering and lattice dynamics, presenting a unique platform for tunable magnetoelectric effects. While experimental observations show that the dielectric constant of this material saturates below 20 K, the application of an external magnetic field induces a dramatic macroscopic dielectric enhancement of approximately 7%. In this study, we elucidate the microscopic origins of this phenomenon using rigorous first-principles Density Functional Theory.

To accurately capture the strong electron correlation and large magnetic moment of the Eu^{2+} ions (S = 7/2), we employ a GGA+U pseudopotentials that explicitly treat the localized $4f^7$ valence electrons. Crucially, we move beyond the simplified cubic approximation by stabilizing the physically accurate I4/mcm antiferrodistortive (AFD) parent phase, ensuring the correct structural anisotropy.

By calculating the total energies of the Ferromagnetic (FM) and G-type Antiferromagentic (G-AFM) configurations, we map the magnetic exchange interactions (J_1,J_2) within the tetragonal lattice. Subsequent Γ-point phonon calculations on the optimized AFD parent phase reveal a doubly degenerate in-plane soft mode responsible for the paraelectric instability. We demonstrate that the transition from the zero-field G-AFM ground state to the field induced FM state directly modulates the spin-dependent hybridization between Eu 4f and O 2p orbitals. This spin-lattice coupling results in a ~3.5% frequency softening of the polar soft mode, perfectly accounting for the experimentally observed 7% dielectric shift. By systematically condensing this imaginary phonon eigenvector to break the I4/mcm symmetry, we map the complete energetic pathway to the polar ground state and offers a robust computational blueprint for predicting magnetoelectric coupling in strongly correlated oxides.

M12 - Recent Developments of the Polaron Theory

M12 – Session 1 (Mon 21, 10:30-12:30, Chair: Serghei Klimin)			
ID	Title	Speaker	Type
457	**Introduction to the minicolloquium "Recent developments of the polaron theory"**	Cesare Franchini; Matthew Houtput; Serghei Klimin; Jacques Tempere	Contributed talk (10:30-10:45)

Cesare Franchini (1) Matthew Houtput (2) Serghei Klimin (3) Jacques Tempere (3)

(1) Computational Materials Physics, University of Vienna, Austria
(2) University of Antwerp
(2) TQC, University of Antwerp, Belgium

The present minicolloquium builds upon and extends a series of successful sessions organized with our participation at previous EPS-CMD Conferences: "Collective Effects and Non-Equilibrium Phenomena in Quantum Gases and Superconductors" (CMD29 – Manchester, 2022), "Quantum Gases as Analogues of Condensed Matter Systems" (CMD30 – Milano, 2023), and "Collective and Nonlinear Phenomena in Confined Quantum Systems" (CMD31 – Braga, 2024).
The concept of polaron has undergone significant broadening relative to its original formulation. Traditional theoretical approaches were largely confined to the linear-harmonic approximation for both the phonon field and the electron–phonon interaction. The inclusion of higher-order terms beyond this approximation can substantially affect the optical response and the kinetics of impurities embedded in crystals. In recent years, sustained efforts along these lines have led to the emergence of the concept of the anharmonic polaron.
While the minicolloquium places particular emphasis on spin-orbit–entangled anharmonic polarons, its scope is not limited to this topic. Rather, it aims to bring together experts working on diverse aspects of polaron physics across a range of media – including crystals, polymers, quantum gases, surfaces, and layered structures – and to highlight recent advances in both methodology and applications of the polaron concept.

697	**Inverse supersymmetry in finite temperature Bose-Fermi mixtures: Connections and differences between the Goldstino and the Polaron**	Carlos Sa de Melo	Invited talk (10:45-11:15)

Carlos Sa de Melo (1)

(1) Georgia Institute of Technology

We investigate nearly degenerate Bose-Fermi mixtures and show that the breaking of generalized supersymmetry (gSUSY) between bosons and fermions, with up to two internal states, manifests itself through the emergence of fermionic Goldstino modes with up to four flavors. In particular, we draw a distinction between typical supersymmetry (SUSY), where bosons have pseudospin 0 and fermions have pseudospin 1/2, and inverse supersymmetry (iSUSY), where bosons have pseudospin 1/2 and fermions have pseudospin 0. In such systems, we highlight that the Goldstino pseudospin is carried by either its constituent fermion (SUSY) or boson (iSUSY). We then distinguish between these two cases by depicting their differing effects on the spectral functions of the bosonic and fermionic atomic species. Furthermore, we propose radio-frequency- or microwave-spectroscopy experiments, analogous to momentum (angular) resolved photoemission in condensed matter physics, to measure the pseudospin-dependent spectral functions and detect the emergence of Goldstino modes in mixtures of 39K and 40K. Lastly, we make connections and point out differences between the Goldstino and the Polaron.

41	**Breakdown of Migdal-Eliashberg theory**	Nikolay Prokofiev	Invited talk (11:15-11:45)

Nikolay Prokofiev (1)

(1) UMass, Amherst

Migdal-Eliashberg theory (MET) describes electrons interacting with phonons in the adiabatic limit when the phonon Debye frequency is much smaller than the Fermi energy. A conventional belief is that MET holds even at strong coupling, when electron self-energy is large, and breaks down only near the point where the dressed phonon spectrum softens to near zero. We analyze numerically and analytically a different option---collapse to a polaronic/bipolaronic ground state. The last scenario has never been analyzed in precise quantitative terms for a generic electron density. We establish rigorous upper bounds on the coupling, at which the Fermi liquid state transforms into the bipolaron (polaron) state, and show that at small and near-maximum densities, this happens well before a dressed phonon softens. This is true both in 2D and 3D systems; in the latter the upper bound on coupling tends to zero (!) in the limit of small or near-full density, indicating that polaron formation cannot be captured by MET and textbook treatment of e-ph problem in continuum is ill-defined. Close to half-filling, the leading instability upon increasing coupling is towards a charge-density-wave.

99	**Approximation-free optical conductivity and mobility of single polaron and finite density polarons by Diagrammatic Monte Carlo**	Andrey S. Mishchenko	Invited talk (11:45-12:15)

Andrey S. Mishchenko (1) Stefano Ragni (1)

(1) Institute of Physics, Zagreb, Croatia

Diagrammatic Monte Carlo (DMC) is the numerical technique of summation of Feynman diagrams without approximations. Bold DMC (BDMC) is the method of self-consistent summation of the irreducible skeleton Feynman diagrams, which are used to modify the Green functions and interparticle interactions by solving the Dyson equation. Modified propagators are used again, forming a self-consistent loop that often circumvents the sign problem in many-body systems.
The DMC was applied to study the optical conductivity (OC) and mobility μ of the single-polaron problem in the Holstein and Frohlich models with linear electron-phonon interaction and the double-well model with highly nonlinear coupling to lattice displacements. The linear models were treated using a DMC

method in momentum space [1,2] and a novel direct-space X-propagator method was developed for the nonlinear model. For every model, one can identify several regimes, some of which are similar across all models. The common feature of all models is the presence of nonmonotonic temperature dependence of μ.
The calculation of OC and μ for systems of finite density was performed by BDMC, which has previously been used to calculate ground-state properties and ARPES of finite-density polaron systems [3,4] . A novel technique, the torn-out polarization operator method, is developed to calculate the current-current correlation function. We describe the method, prove its validity, and show first results of the doping dependence of the optical conductivity and mobility.

[1] A. S. Mishchenko, N. Nagaosa, G. De Filippis, A. de Candia, and V. Cataudella, Phys. Rev. Lett. 114, 146401 (2015).
[2] A. S. Mishchenko, L. Pollet, N. V. Prokof'ev, A. Kumar, D. L. Maslov, and N. Nagaosa, Phys. Rev. Lett. 123, 076601 (2019).
[3] A. S. Mishchenko, N. Nagaosa, and N. Prokof'ev, Phys. Rev. Lett. 113, 166402 (2014).
[4] A. S. Mishchenko, I. S. Tupitsyn, N. Nagaosa, and N. Prokof'ev, Sci. Rep. 11, 9699 (2021).

M12 – Session 2 (Mon 21, 16:00-18:00, Chair: Cesare Franchini)

ID	Title	Speaker	Type
355	**Polarons and Self-Trapped Excitons in Realistic Semiconductors**	Julia Wiktor	Invited talk (16:00-16:30)

Julia Wiktor (1)

(1) Chalmers University of Technology

Carrier localization plays an important role in determining transport and optical properties of functional materials, particularly in soft and polar semiconductors relevant to optoelectronic and energy applications. However, modeling these localized states in realistic materials is not straightforward, because their formation is closely tied to local symmetry breaking, structural fluctuations, and defects. In this talk, I will discuss recent first-principles results on polarons and self-trapped excitons in halide perovskites and $BiVO_4$. I will show how atomistic electronic-structure calculations can be used to identify competing localized states, relate them to spectroscopic signatures, and assess how finite temperature affects their stability and dynamics. Finally, I will highlight recent progress in using machine-learning-based molecular dynamics to describe these phenomena over larger length and time scales.

ID	Title	Speaker	Type
315	**X-Representation Monte Carlo for Polarons in Anharmonic Double-Well Lattices**	Stefano Ragni	Invited talk (16:30-17:00)

Stefano Ragni (1) Tomislav Miškić (1) Thomas Hahn (2) Nikolay Prokof'ev (3) Osor Slaven Barišić (1) Naoto Nagaosa (4) Cesare Franchini (5) Andrey Mishchenko (1)

(1) Institute of Physics, Zagreb, Croatia
(2) Flatiron Institute, New York, USA
(3) University of Massachusetts Amherst
(4) RIKEN Center for Emergent Matter Science
(5) Computational Materials Physics, University of Vienna, Austria

Polaron physics remains central to understanding charge transport in materials with strong electron-phonon coupling, where quasiparticles emerge as electrons dressed by lattice excitations. The Holstein model provides the standard framework for describing small polarons, assuming harmonic phonons and linear coupling. However, this approximation breaks down in materials such as quantum paraelectrics, hydrides, and halide perovskites, where anharmonic lattice effects play a crucial role.
We have developed a continuous-time quantum Monte Carlo method formulated in the ionic displacement basis (X-Representation), which samples the perturbation expansion of the electronic imaginary-time Green's function with respect to electron hopping. The method is approximation-free and enables the treatment of arbitrary anharmonic potentials, including double-well potentials relevant to quantum paraelectrics and ferroelectrics. Moreover, it provides reliable access to the physically relevant adiabatic regime, where phonon frequencies are small compared to electron hopping, and many existing approaches become ineffective.
This talk presents high-precision calculations of ground-state polaron properties across different regimes and combinations of linear and nonlinear electron-phonon coupling, revealing strong renormalization effects in the double-well regime. By extending the method to compute the imaginary-time current-current correlation function, we also extract signatures of the optical conductivity spectrum. These results provide key insights into experimentally observable behavior and highlight the role of anharmonicity in shaping polaron dynamics in complex materials.

ID	Title	Speaker	Type
109	**Analytical approaches to polarons in nonparabolic finite-width conduction bands**	Serghei Klimin	Contributed talk (17:00-17:15)

Serghei Klimin (1) Jacques Tempere (1) Matthew Houtput (1) Ingvar Zappacosta (1) Stefano Ragni (2) Thomas Hahn (3) Lorenzo Celiberti (4) Cesare Franchini (4) Andrey Mishchenko (2)

(1) TQC, University of Antwerp, Belgium
(2) Institute of Physics, Zagreb, Croatia
(3) Flatiron Institute, New York, USA
(4) Computational Materials Physics, University of Vienna, Austria

We develop and compare analytical approaches for the polaron problem in finite-width, non-parabolic conduction bands [1, 2]. Our main result is an extension of the Feynman variational method to tight-binding lattices [1], where the effective-mass approximation breaks down. We also revisit analytical methods originally formulated for continuum polarons, including canonical transformations and improved self-consistent Wigner–Brillouin approximations, and generalize them to lattice systems. In a finite-bandwidth lattice, these approaches exhibit qualitative features absent in the continuum case, such as a nontrivial connection between weak- and strong-coupling limits. An improved Wigner–Brillouin scheme yields a momentum-dependent polaron self-energy free of resonances and consistent with perturbation theory at zero momentum.
The methods are applied to the Holstein model and benchmarked against numerically exact calculations, including Diagrammatic Monte Carlo, exact diagonalization, and density-matrix renormalization-group results, and are further extended to polarons with Rashba spin–orbit coupling.

The self-energy of a Holstein polaron exhibits close agreement between the modified Feynman variational method and numerically exact results. The developed approaches are promising for theoretical study of polarons with different types of the particle-phonon interaction.

[1] S. N. Klimin, J. Tempere, M. Houtput, I. Zappacosta, S. Ragni, T. Hahn, L. Celiberti, C. Franchini and A. S. Mishchenko, arXiv:2603.09609 (2026)
[2] S. N. Klimin, J. Tempere, M. Houtput, S. Ragni, T. Hahn, C. Franchini and A. S. Mishchenko, Phys. Rev. B 110, 075107 (2024).

409	**First principles theory of nonlinear long-range electron-phonon interaction**	Matthew Houtput	Contributed talk (17:15-17:30)

Matthew Houtput (1) Cesare Franchini (2) Serghei Klimin (3) Samuel Poncé (4) Jacques Tempere (3) Ingvar Zappacosta (3)

(1) University of Antwerp
(2) Computational Materials Physics, University of Vienna, Austria
(3) TQC, University of Antwerp, Belgium
(4) Université catholique de Louvain

Electron-phonon interactions are often written using the approximation of linear interaction, where one only keeps the process where one electron interacts with one phonon. This is usually sufficient to quantitatively describe material properties. However, this is no longer true in anharmonic materials with significant electron-phonon interaction, such as quantum paraelectrics and halide perovskites. Currently, the only available models for nonlinear electron-phonon interaction are model Hamiltonians, written in terms of phenomenological parameters. Here, we provide a microscopic semi-analytical expression for the long-range dipole part of the 1-electron-2-phonon matrix element, which can be interfaced with first principles techniques. We show that unlike for the long-range 1-electron-1-phonon interaction, the continuum approximation is not sufficient and that the entire phonon dispersion must be considered. We calculate an expression for the quasiparticle energies and show that they can be written in terms of a 1-electron-2-phonon spectral function. To demonstrate the method in practice, we calculate the 1-electron-2-phonon spectral function for LiF and CsPbI3 from first principles, and we show that the nonlinear interaction contributes significantly to the electron mobility of CsPbI3. The framework presented here bridges the gap between model Hamiltonians and first-principles calculations for the 1-electron-2-phonon interaction.

539	**Relativisistic description of canonical quantization of Josephson effect for the case of superconductor interfaced to semiconductor quantum dots in external magnetic field**	Krzysztof Pomorski	Contributed talk (17:30-17:45)

Krzysztof Pomorski (1,2) Lukasz Stepien (3)

(1) University of New Mexico. Albuquerque, USA
(2) Quantum Hardware Systems, Lodz, Poland
(3) University of the National Education Commission, Krakow

In [1-5] has been investigated a relativistic relation between the Josephson energy and the transport current has been verified. This was further generalized in [6], by including the influence of external charges associated with Wannier-type semiconductor qubits coupled to a Josephson junction. The resulting modification of the Andreev bound states reflects the coupling between the superconducting condensate and the quantum dynamics of the Wannier qubits [7]. Within this framework, we investigate further generalization, i.e. an external magnetic field is swicthed in. A generalized form of the Cooper-pair quasiparticle appears, too. The analysis indicates the emergence of a superposition of effective masses in the generalized superconducting quasiparticle, whose properties can be electrically tuned via the charge states of the nearby Wannier qubits with computational methodology specified in [5-6].

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M12 – Session 3 (Wed 23, 10:30-12:30, Chair: Jacques Tempere)

ID	Title	Speaker	Type
48	**High-throughput analysis of polaron models and variational first-principles approach to self-trapped polarons without supercell**	Xavier Gonze	Invited talk (10:30-11:00)

Xavier Gonze (1)

(1) Université catholique de Louvain

The standard Fröhlich (one phonon band, non-degenerate electronic state, isotropic) model is a workhorse for the large polaron community, used for decades. Recently [1], a generalization of this Fröhlich model (multiple phonon bands, degenerate electronic states, anisotropic) has been introduced.
I will present a high-throughput analysis of the outcome of these two models [2] for a large set of 1260 materials, also analyzing their domain of validity, when fed with first-principles data. mong this extended dataset most materials host perturbative large polarons, but there are many instances that are non-perturbative and/or localize on distances of a few bond lengths. A variety of behaviors is found, with statistical characterization of these for this large set of materials. Then, I will present a first-principles study of self-trapped polaron formation in paradigmatic polar
semiconductors and insulators using the variational polaron equations framework, that does not rely on supercells [3]. The variational approach enables the identification of multiple polaronic states and supports the analysis of polarons with arbitrarily large spatial extent via energy filtering. The potential energy surfaces of the resulting polarons exhibit multiple local minima, reflecting distinct, symmetry-broken polaronic configurations in systems with degenerate band edges.

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708	**Interface-Engineered Coatings (Cu, Sn, and Ag) for Enhanced Flux Pinning and Multi-Filamentary Design in IMD-Processed MgB2 Superconducting Wires**	Ali Gencer	Invited talk (11:00-11:30)

Ali Gencer (1) Fatima Almokdad (1) Fatih Ervuz (1) Chen Guo (2) Haluk Koralay (3) Yanwei Ma (2) Yusuf Oznal (1) Serap Safran (1) Shanli Salahi (3) Ayten Seçkin (3) Kivilcim Sonmez (1) Salih Can Taskin (1) Dongliang Wang (2)

(1) Ankara University, Turkiye
(2) Chinese Academy of Sciences
(3) Gazi University

In this work, MgB2 (with C-coated boron powders) wires were fabricated using the Internal Magnesium Diffusion (IMD) method. To improve flux pinning within the superconducting matrix under applied magnetic fields up to 12 T, the central magnesium rods were coated with different metallic layers, namely Cu, Sn, and Ag, as low-temperature activators. The low-temperature activation effect of Cu coating in IMD-processed MgB2 wires has been previously demonstrated in our earlier work [1]. In the first stage, 200 nm Cu-, Sn-, and Ag-coated MgB2 wires were comparatively investigated to evaluate the effects of metallic activator coatings on MgB2 phase formation and superconducting performance. Subsequently, the effect of Cu coating thickness was further examined by preparing Cu-coated Mg rods with coating thicknesses of 200, 400, 600, and 800 nm, aiming to promote MgB2 formation at lower sintering temperatures and shorter reaction times. In addition, we have found that C-doping of 4% was effective for higher Jc values at low fileds below 7T, while 10% C coating on Boron was very effective in transport Jc measurements at 10 T. Regardless of the origin of Polaron and phonons for the pair mechanism, we will present the effects various dopants for Jc, and Tc performances of the manufactured wires.
The thermal behavior and associated microstructural evolution of the processed Cu-, Sn-, and Ag-coated MgB2 wires were investigated using Differential Thermal Analysis (DTA) and Scanning Electron Microscopy (SEM). Resistance–temperature (R–T) measurements were performed under various applied magnetic fields, and the corresponding superconducting transition behavior, upper critical field (Hc2), and irreversibility field (Hirr) were analyzed. The transport Jc results showed that the highest value among the mono-core wires was obtained for the 200 nm Cu-coated MgB2 wire, reaching 3.9×10^4 A/cm^2 at 4.2 K and 10 T. Finally, based on the optimized Cu activator approach, 7-filament MgB2 wires were fabricated using 200 nm Cu-coated Mg rods, and a Jc value of 1.2×10^5 A/cm^2 was achieved at 4.2 K and 10 T.

179	**Phonon spectral properties of electron–phonon coupled systems**	Osor Slaven Barišić	Contributed talk (11:30-11:45)

Osor Slaven Barišić (1)

(1) Institute of Physics, Zagreb

While often less emphasized than electronic properties, phonon spectral functions provide rich insight into quasiparticles and collective modes involving strong electron–phonon coupling. The hybridization between phonon branches and plasmons has recently been studied [1] to address the superconducting transition temperature in layered materials that host low-energy plasmon modes. Analysis of the phonon spectral function shows that nonadiabatic effects (beyond the Born–Oppenheimer approximation) may significantly enhance the stability of the superconducting phase.
In the dilute limit, the phonon spectral function provides valuable information about the nature of polaron formation. Two physically distinct contributions can be identified [2], both proportional to the polaron concentration: (i) an excess in phonon spectral weight (phonon production), associated with lattice deformation; and (ii) a redistribution of spectral weight toward lower frequencies (phonon softening). In contrast to systems with a finite concentration of itinerant charges, where softening primarily affects phonons at specific momenta, here the softening extends broadly across the Brillouin zone, reflecting the local character of the polaron lattice deformation.

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150	**Quantum-classical study of charge transport in organic semiconductors**	Darko Tanaskovic	Contributed talk (11:45-12:00)

Darko Tanaskovic (1)

(1) Institute of Physics Belgrade

Charge transport in organic semiconductors is limited by electron scattering on thermally excited low-frequency vibrational modes. For these systems, the simple quasiparticle picture underlying the semiclassical Boltzmann approach breaks down, calling for alternative theoretical descriptions. To test the applicability of the quantum-classical (QC) method, which treats the lattice vibrations classically, we first consider the Holstein polaron in one dimension near the adiabatic limit. We calculate the frequency-dependent mobility within the QC method and find very good agreement with the fully quantum solution obtained using the method based on quantum typicality [1]. The most prominent feature is the appearance of a zero-frequency peak in the mobility, in addition to the displaced peak associated to the precursors of Anderson localization. The zero-frequency peak cannot be obtained within the phenomenological transient localization approach, which is often used in a semiquantitative description of charge transport in quasi-one-dimensional organic semiconductors.
We then assess the reliability of the QC approach in more realistic scenarios involving multiple phonon modes in the Holstein model, as well as single-and multimode Peierls models [2]. For parameters relevant to the prototypical organic semiconductor rubrene, we compute the frequency-dependent charge mobility and find excellent agreement with results from the state-of-the-art hierarchical equations of motion method. These results show that the QC method preserves quantitative accuracy in substantially more complex and material-relevant regimes than the single-mode Holstein model. Our microscopic approach complements the phenomenological transient-localization theory and is readily applicable to realistic electron-phonon Hamiltonians.

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[2] D. Tanasković, M. Makrushin, and P. Mitrić, Phys. Rev. B 113, 165108 (2026).

336	**Examining the accuracy of the cumulant expansion method in electron-phonon systems**	Petar Mitrić	Contributed talk (12:00-12:15)

Petar Mitrić (1) Veljko Janković (1) Darko Tanaskovic (1) Nenad Vukmirović (1)

(1) Institute of Physics Belgrade

The cumulant expansion (CE) method provides an alternative to the conventional Dyson equation approach for the calculation of spectral functions and quasiparticle properties in interacting quantum many-particle systems. Furthermore, when combined with the independent particle approximation (IPA), the CE can also be used to calculate charge mobility.
We examine the range of validity of this method by implementing it in simplified model systems—the Holstein, Peierls, and Fröhlich models[1,2]—for which accurate or numerically exact benchmarks are available. Based on these numerical results, supported by analytical arguments using spectral sum rules, we find that for weak to moderate coupling strengths and not-too-low temperatures, the CE within the IPA framework yields accurate results. We also discuss the accuracy of the IPA approximation, i.e., the role of vertex corrections [2,3].

This research was supported by the Science Fund of the Republic of Serbia, Grant No. 5468, Polaron Mobility in Model Systems and Real Materials – PolMoReMa.

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333	**Lattice Bose polarons at strong coupling and quantum criticality**	Alessio Recati	Contributed talk (12:15-12:30)

Alessio Recati (1,2)

(1) Pitaevskii BEC Center, CNR-INO
(2) Università di Trento

We study the physics of an impurity confined in a lattice coupled to a Bose-Hubbard bath at zero temperature. Within the Quantum Gutzwiller formalism [1], we develop a beyond-Fröhlich model of the bath-impurity interaction. Results for the properties of the polaronic quasiparticle due to the dressing of the impurity by quantum fluctuations of the bath are presented throughout the entire phase diagram, focusing on the effect of the Mott-insulator to superfluid quantum phase transition [2]. In the case of strong bath-impurity interaction we develop a new diagrammatic approach based on the quantum Gutzwiller Hamiltonian and the results for the ground state energy is benchmarked via Quantum Monte-Carlo (QMC) calculations [3]. We characterise the modification of the impurity properties due to the presence of the Mott-Superfluid phase transition, and show that the polaron energy shows finite scaling behaviour [4]. Eventually we mention how to realise the dephasing model by coupling a fixed impurity to a Bose-Hubbard model and emphisize the role of an impurity as an unambiguous probe of the quantum criticality of the manybody environment [5].

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M12 – Session 4 (Wed 23, 16:00-18:00, Chair: Matthew Houtput)

ID	Title	Speaker	Type
123	**Hamiltonian renormalization and Fermi liquid theory**	Hadrien Kurkjian	Invited talk (16:00-16:30)

Hadrien Kurkjian (1)

(1) LPTMC - Sorbonne Université & CNRS

I will introduce a new renormalisation scheme to construct the Landau quasiparticles of Fermi fluids. The scheme relies on an energy cutoff Λ which removes the quasi- resonant couplings, enabling the dressing of the particles into quasiparticles via a unitary transformation. The dynamics of the quasiparticles is then restricted to low- energy transitions and is fully determined by an effective Hamiltonian which unifies the Landau interaction function f and the collision amplitude in a single amplitude A regularized by Λ. This effective theory captures all the low-energy physics of Fermi fluids that support Landau quasiparticles, from the equation of state to the transport properties, both in the normal and in the superfluid phase. I will apply it to an atomic Fermi gas with contact interaction.

66	**Ab Initio Theory of Exciton Polarons and Self-Trapped Excitons**	Zhenbang Dai	Invited talk (16:30-17:00)

Zhenbang Dai (1) Feliciano Giustino (1) Jon Lafuente-Bartolome (2) Chao Lian (1)

(1) The University of Texas at Austin
(2) University of the Basque Country UPV/EHU

Excitons, despite being neutral excitations, could interact with the hosting lattice and lead to self-localization, forming exciton polarons or self-trapped excitons. Exciton polarons have been suggested to actively participate in photocatalytic processes, give rise to broadband luminescence, and result in Stokes shift. Furthermore, they could serve as precursors to permanent defects and are thus crucial for quantum technologies. However, the broad interest in the physics of exciton polarons is asymmetric with the scarce ab initio characterizations of this excited-state species, primarily due to the necessity of

using large supercells and the incurred heavy computational cost. In this talk, I will present a supercell-free theory of exciton polarons that is amenable to first-principles calculations. This theory allows us to identify the ubiquitous existence and significant impact of exciton polarons with disparate length-scales in a range of systems, including lithium-ion battery electrode materials, photocatalytic semiconductors, and optoelectronic halide perovskites. I will further demonstrate how this theory can be reduced to a simplified model that sheds light on the formation condition and mechanism of exciton polarons.

This work was conducted in collaboration with Chao Lian, Jon Lafuente-Bartolome, and Feliciano Giustino. This research was primarily supported by the Computational Materials Sciences Program funded by the US Department of Energy, Office of Science, Basic Energy Sciences, under award no. DE-SC0020129. Part of this research was supported by the NSF, Office of Advanced Cyberinfrastructure under Grant No. 2103991 of the Cyberinfrastructure for Sustained Scientific Innovation program, and the NSF Characteristic Science Applications for the Leadership Class Computing Facility program under Grant No. 2139536. This research used resources of the National Energy Research Scientific Computing Center and the Argonne Leadership Computing Facility, which are Department of Energy Office of Science User Facilities supported by the Office of Science of the US Department of Energy, under Contracts Nos. DE-AC02-05CH11231andDE-AC02-06CH11357, respectively. We also acknowledge the Texas Advanced Computing Center at The University of Texas at Austin for providing access to Frontera and Lonestar6.

709	**Interplay Between Laser-Engineered Surface Microstructures and Flux Line Dynamics in YBCO Superconductors**	Fatima Almokdad	Contributed talk (17:00-17:15)

Fatima Almokdad (1) Sait Baris Guner (1) L A Angurel (2) A Badía-Majós (2) G F de la Fuente (2) E Martínez (2) L Porta-Velilla (2) J Rivera-Sahun (2)

(1) Ankara University
(2) Zaragoza University

The interaction between engineered defect structures and the superconducting flux line lattice plays an important role in determining the macroscopic electrodynamic properties of high-Tc cuprates. In this work, we investigate the effects of artificial pinning architectures in top-seeded melt-grown (TSMG) YBCO bulk superconductors. Micro-holes were introduced on the sample surfaces using ultrashort-pulsed (femtosecond) laser irradiation, a technique that operates with minimal microstructural damage typically associated with processing brittle ceramic materials on the order of less than 1 micron. Transport and magnetic measurements indicate that this surface modification alters the magnetic flux distribution and leads to an enhancement in the critical current density (Jc) and the levitation force. Isothermal magnetization (M-H) measurements show a more pronounced second magnetization peak (SMP) in the laser-processed samples compared to pristine ones. The observed enhancement in Jc (H) is discussed in terms of vortex dynamics and pinning, where the laser-induced mesoscopic defects are proposed to act as additional pinning centers, modifying the balance between different vortex creep regimes and possibly extending the stability of disordered vortex phases at higher magnetic fields. These results provide insight into the role of engineered defect landscapes in tuning vortex behavior and improving the performance of YBCO-based bulk superconductors for levitation applications. In addition, we have modelled a search for underlying mechanisms using COMSOL to calculate the mimicking structure resembling the samples used for experimental analysis reported in previously published research work [1]. A detailed comparison will be presented in view of numerically calculated findings of superconducting samples with artificial holes, the microstructure and superconducting properties therein reported.

178	**Variational approach to polaron hopping transport**	Vasilii Vasilchenko	Contributed talk (17:15-17:30)

Vasilii Vasilchenko (1) Matteo Giantomassi (1) Xavier Gonze (1) Samuel Poncé (1)

(1) Université catholique de Louvain

Self-trapped polarons are quasiparticles that form in materials when a free electron or hole becomes localized within a self-induced lattice distortion. This autolocalization can modify the charge transport properties of a system, leading to a transition from band-like transport to thermally activated hopping. Among first-principles approaches to polarons, the Variational Polaron Equations provide an efficient computational framework [1]. As implemented in the ABINIT software package, this approach explicitly treats the polaron-induced charge and structural forces, and enables sampling of the polaron energy landscape across distinct polaronic states. In this contribution, building on this framework, we demonstrate how the explicit treatment of polaron forces enables the variational optimization of minimum energy paths (MEPs) for polaron charge transfer using the string method [2]. Access to multiple polaronic states, together with the MEPs connecting them on the polaron energy landscape, provides a route to estimate hopping mobilities within the framework of transition state theory [3]. These capabilities are demonstrated for rutile TiO_2, a prototypical semiconductor known to exhibit electron polaron self-trapping, whose conductivity measurements display clear signatures of polaronic hopping transport [4].

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40	**Self-Interaction of Polarons through the Piecewise Linearity Condition**	Alfredo Pasquarello	Invited talk (17:30-18:00)

Alfredo Pasquarello (1)

(1) EPFL

The piecewise linearity condition is a property satisfied by the exact density functional and has been found to yield band gaps in accord with experiment when imposed to hybrid functionals [1,2]. Here, we address the self-interaction in relation to polarons in density functional theory. The self-interaction can be corrected by focusing on its one-body form like it appears in Hartree-Fock theory or through the enforcement of the piecewise linearity condition, also referred to as the correction of the many-body self-interaction. We develop a unified theoretical framework encompassing one-body and many-body forms of self-interaction [3,4]. In this way, we establish a quantitative connection between the two forms of self-interaction, by which the many-body form is seen to account for the effect of electron screening [3,4]. Further support for the enforcement of piecewise linearity is provided by the fact that, under this condition, it is possible to unify charged and neutral polaron formulations in density functional theory [5]. In our investigation, we consider widely used functionals such as the global hybrid functional PBE0(α) [3-7], and the Hubbard-corrected functional DFT+U [6,7,8], as well as a newly developed semilocal scheme, called γ-DFT, which involves the use of a weak localized potential [3,4,7]. The enforcement of the piecewise linearity condition is achieved by imposing the generalized Koopmans' condition to the neutral and charged states of the polaron upon proper consideration of finite-size effects induced by the lattice polarization [9]. The polaron properties are found to be robust upon variation of the functional, including charge densities [3-8], structural distortions [3-8], formation energies [3-8], energy barriers [7,8], hyperfine and superhyperfine parameters [7], and charge hopping rates [7].

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M12 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
549 **P014**	**Machine Learning Polaron Dynamics in lithium anode $Li_4Ti_5O_{12}$**	Marco Barducci	Poster

Marco Barducci (1) Cesare Franchini (2) Luca Leoni (1)

(1) University of Bologna
(2) Computational Materials Physics, University of Vienna, Austria

Polarons play a central role in mediating Li-ion diffusion in the $Li_4Ti_5O_{12}$ (LTO) anode. The presence of polarons reduces the energy barrier for Li-ion diffusion and influences both electronic and ionic mobility. However, mobility estimation remains a significant challenge for purely ab initio methods, since the relevant timescales exceed by orders of magnitude those accessible via ab initio molecular dynamics. Machine learning interatomic potentials (MLIPs) provide a promising alternative, combining the accuracy of first-principles methods with substantially reduced computational cost, thus enabling simulations on the nanosecond timescale. In this work, we employ the recently developed MLIP architecture LEOPOLD (Learning of Polaron Dynamics) to estimate the mobility of a single polaron in bulk LTO. This represents a crucial first step toward a broader understanding of polaron dynamics and their impact on Li-ion transport in LTO for battery applications.

ID	Title	Presenter	Type
612 **P015**	**Polaron formation in quantum paraelectric $SrTiO_3$ and $KTaO_3$**	Markus Schwarz	Poster

Markus Schwarz (1) Cesare Franchini (1) Feliciano Giustino (2) Luigi Ranalli (1) Carla Verdi (3)

(1) Computational Materials Physics, University of Vienna, Austria
(2) The University of Texas at Austin
(3) University of Queensland

Recent ab initio calculations for charge transport in $KTaO_3$ and $SrTiO_3$, using the Boltzmann transport equation, showed an overestimated mobility by 300% compared to experimental data [1]. Ab initio polaron calculations for these materials in Ref. [2] showed that localized solutions are possible for an excess electron, hinting towards a polaron transport regime. However, for the supercell sizes used, the localization was confirmed in one spatial dimension only and a full localization was conjectured for larger supercell sizes.
This work further investigates polaron formation in $KTaO_3$ and $SrTiO_3$ based on the ab initio theory of polarons presented in Ref. [3] and implemented in the EPW code [4, 5]. As a result, the conjecture of a large electron polaron localized with respect to all spatial directions was confirmed for both materials. Furthermore, the influence of anharmonic phonons, calculated with the SSCHA code [6], on the formation of an electron polaron was investigated and found to be negligible. Hole polaron calculations yielded consistent results compared to Ref. [2]. Additionally polaron hopping was investigated for a hole polaron in $KTaO_3$.

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ID	Title	Presenter	Type
435 **P016**	**Diagrammatic Monte Carlo for anisotropic and degenerate bands**	Samuele De Amicis	Poster

Samuele De Amicis (1) Cesare Franchini (1) Thomas Hahn (2) Stefano Ragni (3)

(1) Faculty of Physics, Computational Materials Physics, University of Vienna, Kolingasse 14-16, Vienna A-1090, Austria
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The Diagrammatic Monte Carlo (DiagMC) technique has historically been successfully employed to study both large (Fröhlich) and small (Holstein) polarons [1]. A key advantage of DiagMC is its non-perturbative, all-coupling nature, which enables accurate treatment across the entire interaction regime, in contrast to perturbative and variational approaches that are typically limited to weak- and strong-coupling limits, respectively.
However, the Fröhlich and Holstein Hamiltonians are based on simplified assumptions---namely, a single isotropic electron band with quadratic dispersion and a single optical phonon mode with simplified electron--phonon coupling---which are often too restrictive to capture the complex electronic and

vibrational structures of real materials. Extending DiagMC to realistic systems therefore requires overcoming these limitations. In this context, recent developments have introduced fully first-principles DiagMC frameworks [2], marking a significant step forward.
Here, we present DiagMC simulations of large polarons in real materials by relaxing key assumptions of the original models. Using first-principles-based formulations [3,4], we compute energy renormalization, polaron effective masses, dispersion relations, and quasiparticle weights for a range of materials, including AlAs, BaO, CaO, LiF, and TiO^2. We further benchmark our DiagMC results against existing studies based on perturbative and Feynman variational approaches [2,3,4], demonstrating consistency and highlighting the predictive power of the method.

[1] AS Mishchenko et al. “Diagrammatic quantum Monte Carlo study of the Fröhlich polaron”. In: Physical Review B 62.10 (2000), p. 6317.
[2] Yao Luo, Jinsoo Park, and Marco Bernardi. “First-principles diagrammatic Monte Carlo for electron–phonon interactions and polaron”. In: Nature Physics 21.8 (2025), pp. 1275–1282.
[3] Bogdan Guster et al. “Fröhlich polaron effective mass and localization length in cubic materials: Degenerate and anisotropic electronic bands”. In: Physical Review B 104.23 (2021), p. 235123.
[4] Anna Miglio et al. “Predominance of non-adiabatic effects in zero-point renormalization of the electronic band gap”. In: npj Computational Materials 6.1 (2020), p. 167.

M13 - Localization Dynamics in Matter and Waves

M13 – Session 1 (Thu 24, 10:30-12:30, Chair: Masayuki Kimura)			
ID	Title	Speaker	Type
103	**A consistent formulation of electrodynamics and the classical electron without singularities**	Manfried Faber	Invited talk (10:30-11:00)

Manfried Faber (1)

(1) TU Wien

Millikan's famous experiment revealed a contradiction with Maxwell's electrodynamics, which became known as the "4/3 problem" and the "radiation reaction problem". From today's perspective, these issues seem to have been insufficiently understood. The actual origin of the problems lies in the instability of the classical electron. Historical approaches to solving the 4/3 problem require more than three degrees of freedom. In a soliton model, only three field degrees of freedom are required to stabilize a purely electrodynamic electron, as was demonstrated 25 years ago but has largely gone unnoticed until now. Precursors to this model are Dirac's magnetic monopoles and their non-Abelian formulation by Wu-Yang. It is shown how solitons with a size of the classical electron radius can reproduce the electromagnetic cross sections of electrons in Compton, Möller, and Bhabha scattering in agreement with the results of QFT, when the Lorentz contraction is taken into account.

106	**Topological Soliton pairs with long-range Coloumbic interaction**	Rudolf Golubich	Contributed talk (11:00-11:15)

Rudolf Golubich (1)

(1) TU Wien

We determine the interaction potential of a solitonic Positronium in the singlet state, modeled as an SU(2) field, using improved lattice simulations of two solitons at varying separations. The potential is extracted from the energy of the two-soliton configuration as a function of distance. At large separations, the interaction reproduces the classical Coulomb potential quantitatively up to an energy shift $\delta E_\infty \approx 9$ keV of the fitted asymptotic constant relative to $2m_e c_0^2$, assumed to be related to limited numerical precision on the lattice. At shorter distances, deviations from the Coloumb potential of point-like charges appear, that are in qualitative agreement with the asymptotic formula of perturbative Quantum Electrodynamics, reflecting the running of the fine-structure constant, with the inverse fine-structure constant ($\alpha^{-1} \approx 137$) reproduced.

210	**Topological defects in nematic liquid crystals**	Samo Kralj	Invited talk (11:15-11:45)

Samo Kralj (1)

(1) Institute Jozef Stefan

Topological defects (TDs) appear in all systems reached via a symmetry breaking phase transition and are consequently observed at all physical scales, including particle physics, condensed matter and even cosmology. Liquid crystals (LCs) are particularly adequate media to study TDs because they exhibit a rich variety of qualitatively different TDs and in them defects could be relatively easily experimentally observed, e.g., using polarizing microscopy. Of particular recent interest are the so-called twist disclinations in nematic LCs which do not carry the 3D topological charge, however, have nonzero 2D charge. Therefore, in 3D they are not topologically stable. Thus, in ordinary conditions they vanish soon after their creation. However, one can stabilize them energetically by imposing appropriate local orientational frustrations. In the lecture I will present basic properties of twist disclinations and general conditions via which they can be stabilized. Furthermore, I will demonstrate their importance from the perspective of basic physics (they might be analogues of the intriguing neutrinos in particle physics) and applications (they could be exploited as reconfigurable paths for controlled transport of appropriate nanoparticles).

582	**Effective Topological Charge Cancelation Mechanism**	Luka Mesarec	Contributed talk (11:45-12:00)

Luka Mesarec (1) Aleš Iglič (1) Samo Kralj (2)

(1) University of Ljubljana
(2)Institute Jozef Stefan

Topological defects (TDs) arise almost inevitably during phase transitions that involve continuous symmetry breaking. Owing to their topological nature, their essential characteristics are largely independent of microscopic system details, leading to a wide range of universal behaviors. In this work, we present a numerical investigation of TDs in effectively two-dimensional closed soft films with in-plane orientational order, such as liquid crystalline shells and biological membranes. We introduce the Effective Topological Charge Cancellation mechanism, which governs the localized spatial organization of TDs and describes the formation of defect–antidefect pairs on curved surfaces and in the presence of relevant inhomogeneities (e.g., nanoparticles). We define an effective topological charge, incorporating contributions from real, virtual, and curvature-induced (smeared) charges within surface patches characterized by different spatially averaged values of Gaussian curvature. Our results reveal a strong tendency for effective topological charge to go to zero in regions composed of patches with significantly different values of Gaussian curvature. For cases where effective topological charge does not equal to zero, we estimate a critical depinning threshold for defect–antidefect pair formation using an electrostatic analogy.

113	**Soliton molecules and roton-mediated binding in binary condensates**	Russell N. Bisset	Contributed talk (12:00-12:15)

Russell Bisset (1) Chunlei Qu (2) Rene Röhrs (1)

(1) University of Innsbruck
(2) Stevens Institute of Technology

Localized nonlinear excitations can form long-lived bound states whose internal degrees of freedom shape their dynamics. I will present two complementary mechanisms for binding solitary waves in two-component Bose-Einstein condensates and their consequences for localization dynamics.
In miscible, nondipolar mixtures, polarization ("magnetic") solitons interact via an effective potential that supports soliton molecules. This framework identifies the conditions for binding and yields an analytic dissociation energy for oppositely polarized pairs, in agreement with full dynamical simulations.
In dipolar mixtures, a roton minimum of the spin excitation branch induces intersoliton forces that oscillate with separation between dark-antidark pairs. The resulting periodic potential supports multiple bound states at distinct separations and generates spatial spin-density oscillations around individual solitons—both direct signatures of the spin roton. In collisions, dipolar interactions enforce universal low-velocity bouncing, contrasting with the transmit-or-bounce behavior of nondipolar solitons, offering a realistic path to confirming spin rotons experimentally.
These results show how soft spin modes and spin polarization mediate controllable long-range forces that organize the binding and scattering of localized waves.

R. M. V. Röhrs, Chunlei Qu and R. N. Bisset, Phys. Rev. A 112, 053316 (2025)
R. M. V. Röhrs and R. N. Bisset, Phys. Rev. A 113, 033311 (2026)

185	**Two-dimensional spectroscopy of quantum sine-Gordon solitons with ultracold atoms**	Duilio De Santis	Contributed talk (12:15-12:30)

Duilio De Santis (1)

(1) Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

We propose a framework for employing two-dimensional (2D) spectroscopy to investigate the quantum sine-Gordon (QSG) model. Traditionally used to study the structure and dynamics of molecular systems, 2D spectroscopy is increasingly recognized as a powerful tool for exploring collective excitations in quantum many-body physics. By evaluating 2D maps within a Gaussian ansatz, we quantify the QSG system's response to consecutive (time-delayed) perturbations. This approach enables the identification of key features such as the emergence of quantum breather modes, their bound states, signatures of the theory's non-Gaussian nature, and the effects of disorder. Notably, these results are unattainable by means of the traditional linear response paradigm, since the consecutive perturbations bring the system to states with multiple excitations and thus reveal processes such as breather-breather interactions. The computed maps provide detailed insights on the out-of-equilibrium dynamics of the QSG model, which can be experimentally investigated through platforms like ultracold atoms and superconducting qubits. As an example, we examine the implications of our spectroscopic protocol in a system of two one-dimensional tunnel-coupled superfluids within a double-well potential: a natural realization of the QSG model. Furthermore, our framework is generalizable to the study of collective excitations in other paradigmatic quantum many-body systems.

D. De Santis, A. Gómez Salvador, N. Bazhan, S. Erne, M. Prüfer, C. Guarcello, D. Valenti, J. Schmiedmayer, E. Demler, "Momentum-resolved two-dimensional spectroscopy as a probe of nonlinear quantum field dynamics", arXiv:2509.25147 (2025)

M13 – Session 2 (Thu 24, 16:00-18:00, Chairs: Russell Bisset and Xiaoquan Yu)

ID	Title	Speaker	Type
68	**Observations of intrinsic localized modes forming polar nanoregions in a relaxor ferroelectric**	Michael Manley	Invited talk (16:00-16:30)

Michael Manley (1)

(1) Oak Ridge National Laboratory

Relaxor ferroelectrics exhibit broad, diffuse phase transitions, and polar nanoregions (PNRs) in place of the long-range ordering observed in displacive ferroelectrics. While displacive ferroelectrics are explained by the well established soft-phonon theory, a corresponding intrinsic-localized-mode (ILM) theory for relaxors—first introduced by Bussmann-Holder et al. in 2005—has remained elusive experimentally. The challenge largely stems from a "waterfall" effect that obscures the ILM spectral region. In this talk, neutron scattering will be presented on the lead-free uniaxial relaxor ferroelectric strontium barium niobate to reveal evidence of ILMs that form PNRs. In this system the transverse optic (TO) phonon is observed without the waterfall effect, unveiling flat ILM bands below the TO phonon that become increasingly intense upon cooling toward the phase transition and ultimately condense into diffuse elastic scattering associated with PNR formation. Analysis of the ILM intensities supports the idea that they act as a local order parameter for the diffuse relaxor phase transition.

677	**Oscillating ring ferrodark solitons with breathing nematic core in a homogeneous spinor superfluid**	Xiaoquan Yu	Contributed talk (16:30-16:45)

Xiaoquan Yu (1)

(1) China Academy of Engineering Physics

We investigate the dynamics of topological solitons in two-dimensions (2D) and find that a ring ferrodark soliton (FDS) exhibits self-sustained oscillations in a homogeneous quasi-2D ferromagnetic spin-1 Bose-Einstein condensate (BEC), rather than expected indefinite expansion. Moreover, along with the ring radius oscillation, the nematic tensor at the magnetization-vanishing FDS core also exhibits periodic motion.
When the ring radius greatly exceeds the FDS width, the motion is nearly elastic and we derive the ring-radius equation of motion (EOM) which can be recast into a form analogous to the inviscid Rayleigh-Plesset equation for spherical bubbles in classical fluids, but with anomalous terms.
Exact solutions to this equation, as well as the oscillation frequency and amplitude, are obtained analytically. In the absence of the magnetic field, the ring radius and the non-zero eigenvalue of the nematic tensor at the core, i.e., the mass superfluid density, become stationary, while oscillations of the nematic tensor components, driven by the ring curvature, persist at the core. Excellent agreements are found between analytical predictions and numerical simulations.

713	**The Hidden Geometry of Transport in Disordered Matter**	Yann Chalopin	Contributed talk (16:45-17:00)

Yann Chalopin (1)

(1) CNRS - Univ. Paris Saclay

Transport in disordered media is usually described through spectra, eigenmodes, and localization lengths. Yet finite systems are probed point to point: a source excites a specific realization at a specific frequency, and transmission follows sparse, heterogeneous corridors. We show that the resolvent response defines a source-conditioned communication geometry directly on the medium. Its logarithm acts as a transport potential whose basins, ridges, and saddles organize propagation. Within this geometry, attenuation is controlled not by the cumulative cost along a path, but by the minimax saddle: the lowest pass at which source and target first become dynamically connected. This yields a finite-scale constitutive closure for transmission, with subleading corridor and entropic corrections. Tests on disordered graphene and protein elastic networks show that the saddle systematically outperforms path-based predictors, revealing transport as a threshold-controlled, geometric process in finite disordered matter.

620	**Disorder Free Localization**	Rohit Kishan Ray	Invited talk (1:00-17:30)

Rohit Kishan Ray (1)

(1) Virginia Tech

Localization in quantum systems is most commonly associated with disorder: Anderson's seminal result established that quenched randomness in a lattice potential suppresses diffusive transport through destructive interference, a mechanism subsequently extended to the interacting regime by many-body localization theory. Yet localization can emerge in perfectly ordered, translationally symmetric systems when the spectral geometry of the Hamiltonian enforces it---a phenomenon now recognized as disorder-free localization. We begin this talk with an introduction to this mechanism, tracing its appearance across several physical settings: lattice gauge theories with conserved local charges, flat-band systems with macroscopic ground-state degeneracy, and continuous-time quantum walks on fully connected graphs, where maximal connectivity paradoxically confines rather than delocalizes.
We focus on the last of these as a concrete and computationally tractable model. We present an efficient quantum circuit implementation of continuous-time quantum walks that produces disorder-free localization on random graphs from near-full to full connectivity. We then show that localization in this setting can be systematically destroyed by introducing disorder, and that this destruction is controllable. This controllability turns out to be precisely the resource needed to construct quantum batteries from such systems, where disorder acts as a tunable charging mechanism with favorable energetic cost relative to stored ergotropy.

387	**Ergotropy and Dynamical Signatures of Many-Body Localization and Discrete Time Crystals in Disordered Heisenberg Chains**	Francesco Formicola	Contributed talk (17:30-17:45)

Francesco Formicola (1) Vittorio Cataudella (1) Grazia De Bello (1) Giulio De Filippis (1) Donato Farina (1) Carmine Anotnio Perroni (1)

(1) University of Naples Federico II

Many-Body Localization (MBL) and Anderson Localization (AL) represent a fundamental paradigm of non-ergodic quantum dynamics in disordered systems. MBL and AL are hallmarks of interacting and non-interacting systems, respectively. From a quantum-information perspective, MBL phase is uniquely identified by the logarithmic entanglement growth, while in the AL case the entanglement is stationary over time. We investigate anisotropic disordered Heisenberg spin chains through state-of-the-art numerical simulations.
We propose local ergotropy - defined as the maximum work extractable via local unitary operations on a small subsystem - as a robust thermodynamic witness of the transition from the ergodic phase to MBL and AL phases. We demonstrate that within the MBL phase, both local ergotropy, reported in Fig. 1a, and its quantum fluctuations exhibit a slow, logarithmic temporal evolution, mirroring the phenomenology of entanglement entropy. Our findings suggest that leveraging local control provides a novel indicator of localization based on extractable work, offering a thermodynamic alternative to standard entropic measures.
Furthermore, we explore the emergence of discrete time crystals (DTC) when an external drive is applied to such localized systems. A DTC is an out-of-equilibrium phase of matter in which continuous time-translation symmetry is spontaneously broken. As a consequence, the system exhibits a subharmonic response, and observables become periodic with a period that is an integer multiple of that of the drive. Figure 2b shows the imbalance time-correlation function, which exhibits oscillations with a period twice that of the drive and remains coherent over time.
While DTC phases have been extensively studied in Ising-like models, we unveil their robustness in disordered Heisenberg chains . By analyzing the dynamics of ergotropy, entanglement, and spin-spin spatial correlations, we identify clear signatures that characterize the transition from the DTC phase to the MBL regime as the driving parameters are tuned. Our results provide new insights into the stability of out-of-equilibrium phases in many-body quantum systems.

698	**Levy Sachdev-Ye-Kitaev model**	Alexei Andreanov	Contributed talk (17:45-18:00)

Alexei Andreanov (1) Budhaditya Bhattacharjee (2) William Esteban Salazar (3) Dario Rosa (4)

(1) IBS Center for Trapped Ions Quantum Science, Republic of Korea
(2) University of Luxembourg
(3) National University of Singapore
(4) ICTP SAIFR/IFP UNESP

Sachdev-Ye-Kitaev model (SYK) is a paradigmatic quantum disordered many-body model, that is solvable. Its solvability provides multiple insights into physics of many-body interacting quantum problems. The standard model features Gaussian random interactions. Various extensions of the original model were considered in the literature, some solvalbe, others not. The solvable extensions typically inherit the properties of the original SYK. We introduce the Levy Sachdev-Ye-Kitaev model, discuss its solvability and properties. It shows some interesting properties not present in the original SYK, while maintaining solvability.

M13 – Session 3 (Fri 25, 10:30-12:30, Chairs: Yann Chalopin and Alexei Andreanov)			
ID	Title	Speaker	Type
552	**Coherent Interactions Between Discrete Breathers**	Sergej Flach	Invited talk (10:30-11:00)

Lin Deng (1) Weicheng Fu (1,2) Chengguan Fang (1) Sergej Flach (3,4) Liang Huang (1) Yisen Wang (1)

(1) Lanzhou Center for Theoretical Physics
(2) Tianshui Normal University
(3) Institute for Basic Science, Korea University of Science and Technology
(4) Massey University

Discrete breathers (DBs) are spatially localized vibrational modes ubiquitous in physical systems. Despite decades of research, their mutual interactions represent a fundamental yet unexplored facet of nonlinear dynamics. Here we uncover quantitative interaction laws for DB pairs, encoded in tunable energy beating whose amplitude provides a direct coupling metric shaped by energy mismatch, phase configuration, and a separation yielding exponentially decaying, parity-sensitive coupling. The coupling can be strongly modulated by frequency locking, which emerges only under restricted excitation conditions. A minimal nonlinear dimer encapsulates all salient behaviors across diverse lattice models. These results promote DBs from static energy traps to versatile elements for engineering energy transport, tailoring vibrational spectra, and generating acoustic frequency combs.

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768	**Lifetime of breathers in an all flatband latiice**	Juan F.R. Archilla	Contributed talk (11:00-11:15)

Juan Archilla (1) Sergej Flach (2)

(1) Universidad de Sevilla
(2) Institute for Basic Science

A lattice of electrical circuits with some specific coupling and three oscillators per unit cell, called the diamond lattice, has the property that the three phonon bands are optical and completely flat.
The addition of a nonlinear on-site hard potential brings about the existence of breathers, that is localized periodic oscillations. The largest vibration can be located in any of the oscillators inside the unit cell, and their frequencies can be in three of the four different phonon forbidden bands. The forbidden band below the lowest flat band has no breathers due to the hardness of the on-site potential.
There are, therefore, nine different types of breathers, with different properties of stability and energy.
We consider the increase of energy in the different oscillators in a thermalized system, and let the system evolve until thermalization is achieved, measuring the thermalization time. We use a function, called the localization function, which has the property that its value at thermal equilibrium is N/2, where N being the number of oscillators in the system. The different routes to thermalization of the different breathers are described.

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156	**Ballistic energy transport in the nonlinear lattice excited by specific symmetry**	Hiroki Ono	Contributed talk (11:15-11:30)

Hiroki Ono (1) Yusuke Doi (1) Akihiro Nakatani (1)

(1) The University of Osaka

We propose the one dimensional (1D) nonlinear lattice exhibiting ballistic energy transport. The 1D nonlinear lattice is constructed to vanish the umklapp processes which disturb smooth thermal transport. The methodology for construction is based on the symmetry in Fourier space. The nonlinear potential has non-locality, and the strength coefficient of long-range interaction is determined to satisfy the condition of symmetry. We also perform numerical simulation to compute the thermal conductivity in the proposed 1D nonlinear lattice. As a result of numerical simulation, it is shown that the 1D nonlinear lattice supports ballistic energy transport.

324	**Dynamics of localization in two-dimensional nanostructures**	Georgios Kopidakis	Invited talk (11:30-12:00)

Georgios Kopidakis (1)

(1) University of Crete

Two-dimensional (2D) materials of atomic thickness exhibit rich physics and strong potential for advanced technologies. Following the discovery of graphene, extensive research has explored fundamental properties of 2D materials and inspired analogous developments in photonics, cold atoms, and engineered metamaterials. Progress in electronics, optoelectronics, quantum technologies, catalysis, and energy applications highlights the critical role of edge effects. In this context, edge states have emerged as a key factor in understanding and controlling wave propagation in low-dimensional systems. We present theoretical and computational studies, often supported by experiments, on the structural and electronic properties of 2D nanostructures, emphasizing cases where simplified models successfully capture the essential physics. For the well-studied graphene nanoribbons using a tight-binding model with nearest-neighbor interactions, extended to the discrete nonlinear Schrödinger equation to incorporate interaction-induced nonlinearity, we

reveal novel spatially localized states. By analyzing the time evolution of initially localized wave packets, we identify distinct dynamical regimes, ranging from linear spreading to nonlinear self-trapping, or governed by edge geometry and initial conditions. For semiconducting armchair nanoribbons, we demonstrate analytically and numerically the existence of flat band states that remain strictly localized across the ribbon width without spreading along the periodic direction. In zigzag nanoribbons, we construct localized states from partially flat band edge states at the Fermi level, leading to confinement in both transverse and longitudinal directions. The inclusion of strong disorder via random on-site energies results in Anderson localization in all cases. Extensions to related 2D lattices reveal the emergence of robust topological states. These results show that geometry, nonlinearity, disorder, and topology provide multiple localization mechanisms, offering new strategies for controlling transfer of excitations in 2D systems.

Support by S.A.R.F. of the University of Crete, KA11568.

176	**A nonlinear coupled cantilever array with time-periodic on-site potentials and Floquet breathers**	Masayuki Kimura	Contributed talk (12:00-12:15)

Masayuki Kimura (1) Juan Archilla (2) Yusuke Doi (3) Víctor Sánchez-Morcillo (4)

(1) Setsunan University
(2) Universidad de Sevilla
(3) The University of Osaka
(4) Universitat Politècnica de València

Intrinsic localized modes (ILMs) or discrete breathers (DBs) have been observed experimentally in a coupled cantilever array with nonlinear on-site potentials [1,2]. The on-site potential is introduced via the magnetic interaction between a permanent magnet, which is attached to the free end of the cantilever, and an electromagnet. Since the strength of the interaction can be modulated by the current flowing in the electromagnet, it is rather easy to realize a time-dependent on-site potential. Indeed, an ILM was successfully manipulated by locally changing the current of the electromagnet.
In this talk, we briefly introduce the experimental system and the equation of motion. Afterward, DB solutions are obtained for which the on-site potentials are modulated periodically in time. The stability and bifurcations of the DB solutions, namely Floquet breathers [3], will be discussed.

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[1] M. Kimura, T. Hikihara, “Coupled Cantilever Array with Tunable On-site Nonlinearity and Observation of Localized Oscillations,” Phys. Lett. A 373, 1257-1260 (2009).
[2] M. Kimura, T. Hikihara, “Experimental Manipulation of Intrinsic Localized Modes in Macro-Mechanical System,” Nonlinear Theory and Its Applications, IEICE 3(2), 233-245 (2012).
[3] M. Kimura, Juan F.R. Archilla, Y. Doi, V.S. Sánchez-Morcillo, “Floquet breathers in a modulated nonlinear lattice,” Chaos 36, 033151 (2026).

38	**Floquet breathers in a time-modulated nonlinear lattice**	Juan F.R. Archilla	Contributed talk (12:15-12:30)

Juan Archilla (1) Masayuki Kimura (2) Yusuke Doi (3) Víctor Sánchez-Morcillo (4)

(1) Universidad de Sevilla
(2) Setsunan University
(3) The University of Osaka
(4) Universitat Politècnica de València

Floquet discrete breathers are localized periodic solutions that may appear in nonlinear lattices with periodic modulation in space and time.
Based in a previous experimental device constructed with cantilevers and with additive time-periodic excitation, we have designed a system with parametric driving that can be modulated in space and time.
For that system, we deduce theoretically the changes brought about by the modulation, first in the phonon band and then on breather properties as existence, stability and the numerical methods to obtain them.
We have found a large variety of Floquet breathers with equal period of the modulating one, multiplied or divided by an integer and communsurate ones.
The results are applicable to a variety of systems and are not limited to the specific model.

JFRA acknoledges a travel grant from Universidad de Sevilla, VII PPITUS-2026 and project PID2022-138321NB-C22 funded by MICIU/AEI/10.13039/501100011033 and ERDF/EU.
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M14 - Experimental Studies of Negatively Charged Ions

M14 – Session 1 (Mon 21, 10:30-12:30)			
ID	Title	Speaker	Type
545	**Infrared action spectroscopy of molecular anions**	Sandra Brünken	Invited talk (10:30-11:00)

Sandra Brünken (1,2) Prateek Boga (1,2) Franziska Dahlmann (3) Katrin Erath-Dulitz (4) Pavol Jusko (5) Stephan Schlemmer (6) Roland Wester (4)

(1) HFML-FELIX
(2) Radboud University
(3) KTH Royal Institute of Technology
(4) Universität Innsbruck, Department of Ion Physics and Applied Physics
(5) MPE Garching
(5) I. Physikalisches Institut, Universität zu Köln

The discovery of molecular anions in the interstellar medium nearly 20 years ago has profoundly changed our understanding of astrochemical networks. The radio-astronomical identification of carbon-chain and nitrile anions such as C_8H^- and C_3N^- has revealed that anions can reach appreciable abundances in cold interstellar environments. In addition to interstellar and circumstellar sources, molecular anions have also been detected in the atmosphere of Titan. These discoveries have triggered extensive experimental and theoretical studies in the last decades on their spectroscopy, formation pathways, reactivity, and destruction mechanisms, significantly advancing our understanding of their role in an astrochemical and astrophysical context.
Laboratory rotational spectroscopy has in the past been essential in providing the precise transition frequencies required for astronomical detection. More recently, infrared action spectroscopy of mass-selected anions has emerged as a powerful complementary approach, with the potential to provide laboratory reference data for their infrared detection, e.g., with the James Webb Space Telescope. The focus of this talk will be on experiments at the FELion cryogenic ion trap beamline at HFML-FELIX which enables broadband, high-sensitivity vibrational spectroscopy of cold ions using the intense and widely tunable FELIX free-electron lasers. They provide detailed structural fingerprints and allow the characterization of transient or weakly bound species inaccessible to conventional methods. Applications extend to a wide range of astrochemically relevant anions, including hydrocarbons, nitriles, halogen-containing species, and polycyclic aromatic hydrocarbon (PAH) anions. These experiments, employing infrared-predissociation spectroscopy at cryogenic temperatures, yield vibrational spectra that can be directly compared with quantum-chemicalcalculations and astronomical infrared signatures.

433	**Negative ion studies at the Cryogenic Storage Ring (CSR)**	Viviane C. Schmidt	Invited talk (11:00-11:30)

Viviane C. Schmidt (1,2)

(1) Institut für Ionenphysik und Angewandte Physik, Universität Innsbruck, Austria
(2) Max-Planck-Institut für Kernphysik, Heidelberg, Germany

Molecules offer a variety of excitation possibilities through their electronic, vibrational and rotational degrees of freedom. The coupling between those modes and consequentially the corresponding decay rates range from atomic timescales to hours and beyond. Negatively charged species are especially well suited to study these mechanisms as their excess electron is typically loosely bound and can be employed as a sensitive probe of the system's internal excitation. Spontaneous auto-detachment or photo-induced action spectroscopy have proven powerful methods to gain insights into the internal relaxation processes of excited anionic species.
The electrostatic Cryogenic Storage Ring (CSR) [1] in Heidelberg provides ideal conditions for such studies. Due to a closed-cycle liquid helium system, temperatures below 10K and residual gas pressures below 10 particles/cm can be reached inside the experimental chambers of the 35m-circumference ring. As a result, ions can be stored and studied for hours in an environment with negligible interference from residual gas collisions and background radiation. Under such conditions, systems with a permanent dipole moment will cool down to their lowest ro-vibrational states. The CSR is equipped with a number of experimental stations. Here, the stored ions can be overlapped with well-defined reactant beams of electrons, photons or neutral particles to study reactions under interstellar conditions.
This talk will introduce the CSR facility before focusing on studies of negative ion species. These include the auto-detachment of highly excited C
and its strong dependence on the system's rotational excitation [2,3]. Furthermore, the validity of the harmonic cascade model used to describe the radiative cooling of isolated molecules was tested using aluminum clusters [4]. Additional studies on negative ions are currently ongoing.

[1] R. von Hahn et al., Rev. Sci. Instrum., 87, 063115 (2016)
[2] V. C. Schmidt et al., Phys. Rev. Lett. 133, 183001 (2024)
[3] V. C. Schmidt et al., Phys. Rev. A 110, 042828 (2024)
[4] Y. Shabo et al., Phys. Chem. Chem. Phys. (2026)

781	**Near-threshold photodetachment of WF_5^- molecular anions in a cryogenic storage ring**	Hubert Gnaser	Contributed talk (11:30-11:45)

Hubert Gnaser (1) Martin Martschini (1) Robin Golser (1) David Leimbach (2) Dag Hanstorp (2) Mingchao Ji (3) Paul Martini (3) Ansgar Simonsson (3) Rachel Poulose (3) Mikael Björkhage (3) Henning Zettergren (3) Henning T. Schmidt (3)

(1) Universität Wien
(2) University of Gothenburg
(3) Stockholm University

The photo-induced detachment of WF_5^- molecular anions was investigated in the Double ElectroStatic Ion Ring ExpEriment (DESIREE) [1] for photon energies from 2.5 eV to 4.5 eV, using an OPO laser system for excitation. This energy range covers the threshold for the removal of an electron from that anion species. Photo-induced reactions were observed which indicate the existence of an energy threshold for WF_5^- anions above which the neutralization yield increases strongly. In that range, the data of the neutral signal could be fitted by a linear function of photon energy E, resulting in a threshold energy E_{th} = 3.130.01 eV. In addition, spontaneous decay processes were observed over time scales of several tens of ms [2]. In accelerator mass spectrometry, this possible suppression of WF_5^- anions by photodetachment could be very beneficial for the efficient detection of the extremely rare radioisotope ^{182}Hf using the $^{182}WF_5^-$ analyte anion; for this, the WF_5^- anion constitutes a pronounced stable interfering isobar [3].The radionuclide ^{182}Hf is of great relevance in

astrophysical environments as it constitutes a potential candidate to study events of nucleosynthesis that may have taken place in the vicinity of the solar system several million years ago.

[1] H. T. Schmidt, et. al., Rev. Sci. Instrum. 84, 055115 (2013).
[2] H. Gnaser, el. al., J. Chem. Phys. 157, 044304 (2022).
[3] M. Martschini, et. al., Radiocarbon 64, 555 (2022).

658	**Mutual neutralization reactions in a cryogenic ion trap**	Maximilian MŠrk	Contributed talk (11:45-12:00)

Maximilian Märk (1) Michael Hauck (1) Roland Wester (1) Robert Wild (1)

(1) Universität Innsbruck, Department of Ion Physics and Applied Physics

Many studies are available discussing ion-neutral reactions at low temperatures, while mutual neutralization reactions (MN) are still experimentally rare. However, these anion-cation reactions play a crucial role in the chemistry of the interstellar medium. Models of these clouds rely heavily on their reaction rate coefficients [T. J. Millar et al., Chem. Rev. 117, (2017)]. In the literature the majority of these reactions are assigned the same rate coefficient, which is an approximation [N. S. Shuman et al., J. Phys.: Conf. Ser. 300 (2011)]. We will address this by measuring MN reactions of abundant ions in the interstellar space. Additionally, these systems can be used for benchmarking theoretical calculations of MN reactions [M. Roy et al., J. Chem. Phys., 2025]. To achieve this, we will utilize our cryogenic 16-pole wire trap, which is designed to create a relatively flat potential with steep walls [M. Nötzold et al., Phys. Rev. A, 106 (2022)]. The wires of the trap are driven with an RF voltage to contain the ions radially. A DC voltage is usually applied to endcap electrodes for axial confinement, but this only works for one charge polarity at a time. To investigate MN reactions, we will also drive the axial confinement using an RF voltage. With this trap we control the temperature and density to simulate different environments. The large expected cross section due to the attractive Coulomb potential will be offset by the low densities in the ion trap. Therefore, long storage times are essential. Our group has already demonstrated long trapping lifetimes for three-body reaction studies [C. Lochmann et al., J. Phys. Chem. A, 127 (2023)]. The status of the experiment will be reported.

647	**Isobar separation for actinide anion beams in AMS**	Andreas Wiederin	Contributed talk (12:00-12:15)

Andreas Wiederin (1) Martin Martschini (1) Peter Steier (1) Karin Hain (1)

(1) University of Vienna

Isobaric interferences have restricted the applicability of Accelerator Mass Spectrometry (AMS) for ultra-trace measurements to certain long-lived radionuclides up to the mid-mass range of fission products or whose isobars do not form negative ions. We investigated two methods to extend isobar separation capabilities to the actinides based on the formation of and interactions with negative ion beams. Anion Formation Isobar Analysis (AFIA) utilizes element-specific AnF_4^-/AnF_5^- (An = U, Np, Pu, Am) formation ratios in a Cs-sputter ion source. These ratios differ by an order of magnitude between adjacent actinides; significant interference thus results in a measurable deviation. While AFIA provided a first isobar screening capability, it is susceptible to false positives from complex isobar mixtures. By contrast, Ion-Laser InterAction Mass Spectrometry (ILIAMS) provides higher sensitivity and reliable results independent of sample composition. The anion beam is decelerated in a gas-filled radiofrequency quadrupole ion guide for residence times of milliseconds. Then, high-powered lasers or reactive gases can be used to selectively suppress isobars. We demonstrated selective UF_4^- removal by a 637 nm laser. Alternatively, adding 3% O_2 to the He buffer gas suppresses both UF_4^- and NpF_4^-, but not PuF_4^-. This approach enabled the preliminary analysis and validation of a ^{236}Np isotopic spike, facilitating AMS measurements of the anthropogenic actinide ^{237}Np. Further isobar separation schemes have been explored for the measurements of ^{241}Pu, ^{241}Am and – if combined with robust chemical separation of ^{238}U - even ^{238}Pu. These radionuclides can provide important source term or age information for environmental samples.

The research was supported by the Austrian Science Fund grant I 4803-N and a Dimitrov Fellowship of the Austrian Academy of Sciences.

636	**Low temperature ultraviolet photodissociation spectroscopy of [dAMP-H]$^-$**	Christian Sprenger	Contributed talk (12:15-12:30)

Christian Sprenger (1) Franziska Dahlmann (2) Eric Sebastien Endres (1) Sunil Kumar S (3) Salvi Mohandas (3) Uma Namangalam (3) Gabriel Schöpfer (1) Roland Wester (1k) Miriam Westermeier (1) Samuel White (1)

(1) Universität Innsbruck
(2) KTH Royal Institute of Technology, Stockholm
(3) IISER Tirupati

To deepen the understanding of photoexcitation of DNA by ultraviolet radiation, we performed a wavelength dependent photoabsorption study of the anionic deprotonated nucleotide $[dAMP-H]^-$. Within the range of our study, between 240 nm and 270 nm, we were able to resolve multiple spectral features, that could not be resolved before. This was made possible by our 16-pole radiofrequency wire trap, which operates at a temperature of 3 K. Furthermore we analysed the yield of five ionic photofragments as a function of wavelength. Finally we determined the absolute photfragmentation cross section of $[dAMP-H]^-$, by performing a comparative measurement of the I^- photodetachment cross section. The results of these photodissociation measurements, published in [1], will be presented.

[1] C. Sprenger, S. J. M. White, M. Westermeier, G. Schöpfer, F. Dahlmann, U. Namangalam, S. Mohandas, S. Kumar S, E. S. Endres, M. Onćak, R. Wester, J. Phys. Chem. A, (2025) 129, 50, 11571-11579

M15 - Light-Wave Driven Dynamics in Quantum Materials

M15 – Session 1 (Thu 24, 16:00-18:00, Chair: Anna Galler)			
ID	Title	Speaker	Type
50	**Peering into topological phases with attosecond spectroscopy**	Antonio Picón	Invited talk (16:00-16:30)

Antonio Picón (1)

(1) Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC)

Attosecond transient absorption and reflectivity spectroscopy provide direct access to electron motion in quantum materials, enabling the study of light induced phases with unprecedented temporal resolution and offering a route to elucidate the role of electron correlations in ultrafast transient phases. In many experiments, however, the spectral response is dominated by the dynamical Franz-Keldysh effect, which arises from the coherent motion of light-driven electrons. Despite its prominence, this response also contains subtle information about the underlying topological structure of the system.
Here, we present a numerical study of a Chern insulator whose topological character is controlled through second-order hopping terms. We simulate the nonequilibrium electron dynamics driven by a circularly polarized infrared pump and probed by an ultrafast attosecond x-ray pulse [1]. Our results reveal a pronounced laser-induced dichroism that provides a clear spectral signature of the topological phase. By analyzing this dichroism, we establish a direct connection between the observed spectral features and the Berry curvature distribution of the material.
These findings demonstrate that attosecond absorption spectroscopy can be leveraged to detect and characterize nontrivial topological phases. This work opens new avenues for probing quantum materials through laser-driven electron dynamics and highlights attosecond techniques as a potential tool to investigate the topological phase structure.

[1] Juan F P Mosquera et al., Rep. Prog. Phys. 87, 117901 (2024)

ID	Title	Speaker	Type
260	**Direct subcycle momentum-resolved observation of lightwave-driven Landau-Zener-Majorana transitions in graphene**	Giacomo Inzani	Contributed talk (16:30-16:45)

Giacomo Inzani (1) Vincent Eggers (1) Manuel Meierhofer (1) Lasse Münster (1) Jakob Helml (1) Robert Wallauer (2) Sarah Zajusch (2) Suguru Ito (2) Leon Machtl (1) Hao Yin (3) Christian Kumpf (3) Francois C. Bocquet (3) Changhua Bao (1) Jens Güdde (2) F. Stefan Tautz (3) Rupert Huber (1) Ulrich Höfer (1,2)

(1) Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN), University of Regensburg
(2) Department of Physics, Philipps-Universität Marburg
(3) Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich

The ultrafast acceleration of electrons in solids by atomically strong light fields forms the basis of lightwave electronics [1,2]. When the field exceeds the adiabatic regime, non-adiabatic Landau–Zener–Majorana (LZM) tunnelling drives interband transitions at optical clock rates [3,4]. Graphene, with its Dirac-like dispersion and high damage threshold, is an ideal platform to study these effects, yet their direct observation remains challenging due to the need of both attosecond temporal resolution and full momentum-space access.
Here, we introduce subcycle band-structure videography across the entire first Brillouin zone, enabling direct tracking of lightwave-driven carrier dynamics with attosecond precision. Using intense few-cycle mid-infrared fields, we resolve the interplay of inter- and intraband processes in graphene. Coherent intraband acceleration and periodic LZM tunnelling induce characteristic modulations of the electron distribution in momentum space at the fundamental and second-harmonic frequencies of the driving field. At later times, carrier redistribution and thermalization indicate the gradual loss of coherence, marking the transition from single-particle to scattering-dominated many-body dynamics [5]. Our photoemission-based approach provides the first direct visualization of strongly driven electrons in full two-dimensional momentum space. It reveals how field-driven acceleration and interband coupling govern Dirac fermion motion and identifies scattering as the key limit to coherent evolution. These results uncover the microscopic dynamics of LZM tunnelling and mark a step toward coherent lightwave control in quantum materials and future petahertz electronics [1,2].

[1] Borsch et al., Nat. Rev. Mater. 8, 668 (2023).
[2] Ossiander et al., Nat. Commun. 13, 1620 (2022).
[3] Higuchi et al., Nature 550, 224 (2017).
[4] Boolakee et al., Nature 605, 251 (2022).
[5] Eggers et al., arXiv preprint arXiv:2602.12844 (2026).

ID	Title	Speaker	Type
172	**Probing Broken Time-Reversal Symmetry in 2D Materials with Tailored-Light Photocurrent Generation**	Selina Nöcker	Contributed talk (16:45-17:00)

Peter Hommelhoff (1,2) Daniel Lesko (1,2) Ofer Neufeld (3) Weizhe Li (1) Selina Nöcker (1,2) Tobias Weitz () Simon Wittigschlager (1)

(1) Department of Physics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU)
(2) Fakultät für Physik, Ludwig-Maximilians-Universität, München
(3) Technion Israel Institute of Technology

Symmetry breaking underpins a wide range of nonlinear physical phenomena [1–4]. Specifically, tailored light–matter interactions with graphene, a highly symmetric two dimensional material, provide a powerful platform for probing such symmetry breaking through photocurrent spectroscopy. Using two linearly polarized harmonic fields with independent control over relative polarization angle and temporal delay, we systematically map photocurrent selection rules arising from the interplay of the driving field and the material symmetries [2,5,6]. In inversion-symmetric graphene, two-color photocurrents predominantly originate from injection currents associated with asymmetric carrier populations in the conduction bands. Time-reversal symmetry (TRS) enforces equal excitation probabilities at conjugate momenta, resulting in symmetry-protected suppression of injection currents when TRS is preserved. Using biharmonic field synthesis, we selectively break or maintain TRS and mirror symmetry, enabling direct identification of symmetry-dependent current suppression and phase-dependent photocurrent generation. Our experimental results are quantitatively benchmarked against state-of-the-art time-dependent density functional theory (TDDFT) simulations. We further extend this approach to systems with intrinsically broken TRS, including the magnetic van der Waals material CrI and an inversion-symmetric Floquet topological insulator. Simulated two-color photocurrent responses in these systems exhibit qualitatively distinct phase dependencies, highlighting the sensitivity of this method to underlying symmetry properties. Overall, our work establishes

photocurrent suppression of ultrafast, linearly polarized two-color fields as a direct, versatile and noninvasive probe of symmetry-broken phases of matter, without the need for magnetic fields or circularly polarized light [7].

[1] D. Ayuso et al., Nat. Photonics 13, 866-871 (2019).
[2] O. Neufeld et al., Phys. Rev. Lett. 127, 126601 (2021).
[3] D. Habibović et al., Nat. Rev. Phys. 6, 663-675 (2024).
[4] O. Neufeld, ACS Photonics (2025).
[5] I. Franco and P. Brumer, J. Phys. B: At. Mol. Opt. Phys. 41, 074003 (2008).
[6] M. Shapiro and P. Brumer, ISBN 9783527409044 (2011).
[7] D. M. B. Lesko et al., ACS Nano (2026)

224	**Lightwave manipulation of magnetism with tailored light: Towards Petahertz spintronics from broken symmetries**	Ofer Neufeld	Invited talk (17:00-17:30)

Ofer Neufeld (1)

(1) Technion Israel Institute of Technology

Recently, ultrafast electron dynamics have been successfully controlled, and measured, with intense femtosecond lasers. This has enabled attosecond probing of many fundamental physical phenomena and material properties and should advance petahertz scale electronic devices with Lightwave coherent manipulation. At the same time, the field of ultrafast magnetism has rapidly evolved, enabling analogous types of coherent control directives, but for electronic spins. Such control can be employed for spin transfer protocols, optical magnetic switches, Lightwave magnetic phase manipulation, and spin currents for spintronics. In principle, this allows merging strong-field-induced electron dynamics with spin dynamics, enabling Petahertz spintronics. I will briefly introduce the prospects and motivation for the field. Subsequently, I will review our recent advancements in these directions. First, I will present ab-initio predictions for CEP-controlled transient magnetic phases driven by intense few-cycle lasers in initially non-magnetic materials. I will next show that by using few-cycle lasers with inherently broken time-reversal symmetry, magnetization can be generated even with linearly-polarized pulses. By introducing two-color tailored laser driving, the out-of-plane magnetization generated in 2D materials can be coherently rotated into 3D spin dynamics control, enabling a wider array of available magnetic phases. This effect arises by precise symmetry breaking in tailored two-color fields that manipulates mirror symmetries, time-reversal symmetry, and inversion symmetry, all of which play a critical role in photocurrent generation and spin dynamics (which I will show are intimately related phenomena). Lastly, I'll introduce measures for evaluating the degree of these symmetry breakings in a tailored laser field, which can also be employed for ultrafast magnetic phase detection.

186	**Giant dynamical paramagnetism in light-driven pseudogap YBCO**	Duilio De Santis	Contributed talk (17:30-17:45)

Duilio De Santis (1)

(1) Institute for Theoretical Physics, ETH Zurich, 8093 Zurich, Switzerland

Superconducting-like behaviors have been observed, in the past decade, in various materials under intense pump fields. In the cuprate $YBa_2Cu_2O_{6+x}$ (YBCO), such remarkable effects have been reported up to the pseudogap temperature. Recently, a transient magnetic field proportional to and aligned with an external field was measured in a breakthrough experiment with pumped YBCO, suggesting flux expulsion via the Meissner effect. We discuss an alternative explanation, based on the idea that the pump-induced, far-from-equilibrium dynamics of YBCO reveals short range superconducting correlations in equilibrium much more dramatically than traditional perturbative probes. Under optical pumping, the system evolves according to a driven sine-Gordon equation, which exhibits a novel instability in the presence of an external magnetic field. This phenomenon leads to a giant paramagnetic magnetization in the same direction as the external field. Results of the theoretical model are in quantitative agreement with the experimental data. The driven YBCO experiment thus has the important consequence of revealing the presence of local pairing in the pseudogap phase. More broadly, the observed instability constitutes a new mechanism for amplifying external magnetic fields at ultrafast time scales.

M. H. Michael, D. De Santis, E. A. Demler, P. A. Lee, "Giant Dynamical Paramagnetism in the driven pseudogap phase of $YBa_2Cu_2O_{6+x}$", arXiv:2410.12919v1 (2024)

148	**Nuclear electric resonance and vibrationally induced magnetism: Strategies for nuclear-spin-based, optical quantum control off the mainstream**	Andreas W. Hauser	Contributed talk (17:45-18:00)

Matthias Diez (1) Andreas W. Hauser (1) Albert Hirtenfelder (1) Johannes K. Krondorfer (1)

(1) Graz University of Technology

Nuclear spin state manipulation is of particular interest for quantum control due to the comparably large coherence times in this degree of freedom. While spin manipulation and detection via magnetic resonance is a standard procedure for large ensembles, the selective addressing of a single nuclear spin, located at a specific position, is highly problematic from the perspective of classical nuclear magnetic resonance.
In this talk, two alternative, light-based pathways are presented, which have been proposed by us recently. The first method employs the nuclear electric quadrupole moment of aspherical nuclei as a handle to access nuclear spin states through time-dependent electric fields. [1,2,3] The second method identifies the vibrational excitation of pseudorotational motions in suitable, highly symmetric molecules as a possible way to generate localized magnetic fields, [4,5] and is closely related to the phenomenon of phonon-mediated dynamical multiferroicity, [6,7] where a time-dependent polarization is linked to magnetization in bulk materials.
Both methods have in common, that they aim for a link between highly developed and well established technologies, such as microelectronics and quantum optics, and nuclear spin systems. On the long run, by introducing pulsed lasers in the optical or IR regime as a tool for spin control, the long coherence times of the nuclear spin degrees of freedom might become accessible via known and proven technology standards.

1 J. K. Krondorfer and A. W. Hauser. Nuclear electric resonance for spatially resolved spin control via pulsed optical excitation in the UV-visible spectrum. Phys. Rev. A, 108:053110, 2023.
2 J. K. Krondorfer, M. Diez, and A. W. Hauser. Optical Nuclear Electric Resonance in LiNa: Selective Addressing of Nuclear Spins through Pulsed Lasers. Physica Scripta, 99:075307, 2024.
3 J. K. Krondorfer, S. Pucher, M. Diez, S. Blatt and A. W. Hauser. Optical nuclear electric resonance as single qubit gate for trapped neutral atoms. J. Phys. B: At. Mol. Opt. Phys. 58:235001, 2025.

4 R. Wilhelmer, M. Diez, J. K. Krondorfer, and A. W. Hauser. Molecular Pseudorotation in Phthalocyanines as a Tool for Magnetic Field Control at the Nanoscale. Journal of the American Chemical Society, 146(21):14620–14632, 2024.
5 M. Diez, J. K. Krondorfer, A. Hirtenfelder and A. W. Hauser. Magnetic coupling between nuclear motion and nuclear spins in molecules. Molecular Physics, e2600464, 2025.
6 D. M. Juraschek, M. Fechner, A. V. Balatsky, and N. A. Spaldin. Dynamical multiferroicity. Phys. Rev. Materials, 1:014401, Jun 2017.
7 D. M. Juraschek and N. A. Spaldin. Orbital magnetic moments of phonons. Phys. Rev. Materials, 3:064405, Jun 2019.

M15 – Session 2 (Fri 25, 10:30-12:30, Chair: Marcus Ossiander)

ID	Title	Speaker	Type
758	**Squeezed light from strongly-driven η-pairing states in the Hubbard model**	Denitsa Baykusheva	Invited talk (10:30-11:00)

Denitsa Baykusheva (1)

(1) Institute of Science and Technology Austria

High-harmonic generation in correlated electronic systems has recently emerged as a sensitive probe of many-body interactions [1,2]. Still, the question on how long-range electronic coherence leaves its imprint on the emitted light and its photon statistics [3,4] remains largely unaddressed. η-pairing states [5] in the half-filled Hubbard model represent exact eigenstates exhibiting off-diagonal long-range order. Here we investigate how η-pairing correlations reshape the strong-field emission. We find pronounced differences compared to the Mott-insulating ground state in both the intensity and the photon statistics of the emitted field, accompanied by a pronounced squeezing of the harmonic emission in the η-state. This indicates that the statistical features of HHG carry diagnostic information about electronic order beyond what power spectra alone reveal. Finally, I will report on experimental progress towards experimental detection of the imprints of electronic correlations in the photon statistics of the emitted harmonics.

[1] Silva et al., "High-harmonic spectroscopy of ultrafast many-body dynamics in strongly correlated systems", Nat. Photonics 12, 266–270 (2018)
[2] Murakami et al., "High-Harmonic Generation in Mott Insulators", Phys. Rev. Lett. 121, 057405 (2018).
[3] Lange et al., "Electron-correlation-induced nonclassicality of light from high-order harmonic generation", Phys. Rev. A 109, 033110 (2024)
[4] Lange et al., "Excitonic Enhancement of Squeezed Light in Quantum-Optical High-Harmonic Generation from a Mott Insulator", Phys. Rev. Lett. 135, 043603 (2025)
[5] Yang et al., "η-pairing and off-diagonal long-range order in a Hubbard model", Phys. Rev. Lett. 63, 2144–2147 (1989)

ID	Title	Speaker	Type
214	Ultrafast dynamics and light-induced superconductivity from first principles	Dominik Spath	Contributed talk (11:00-11:15)

Alejandro Simon (1) Emma Batson (1) Karl Berggren (1) Pedro N. Ferreira (2) Reed Foster (1y) Christoph Heil (2) Phillip D. Keathley (1) Eva Kogler (2) Rohit Prasankumar (3) Mihir Sahoo (2) James Shi (1) Dominik Spath (2)

(1) Research Laboratory of Electronics, Massachusetts Institute of Technology
(2) Institute of Theoretical and Computational Physics, Graz University of Technology
(3) Deep Science Fund, Intellectual Ventures

Ultrafast light fields provide a powerful technique for driving quantum materials far from equilibrium, yet achieving a predictive, microscopic description of their dynamics remains a major challenge. In this talk, I will present a new first-principles framework for optically driven superconductors that directly connects microscopic electron–phonon interactions to time-resolved experimental observables. By solving the Migdal–Eliashberg equations directly on the real-frequency axis and coupling them to nonequilibrium kinetics, we capture the evolution of quasiparticles, phonons, and optical response in driven materials [1, 2].
We demonstrate quantitative agreement with ultrafast optical measurements in superconducting Pb and high-pressure LaH_{10}, accurately reproducing both the amplitude and timescales of the measured transient response across very different electron–phonon regimes. Building on this validation, we apply the method to light-driven systems and identify a potential mechanism for transient superconducting enhancement arising from resonant quasiparticle redistribution [2].

[1] Simon et al., Fast real-axis Eliashberg calculations: Full-bandwidth solutions beyond the constant density of states approximation, arXiv (2026)
[2] Simon et al., Ultrafast dynamics and light-induced superconductivity from first principles, arXiv (2026).

ID	Title	Speaker	Type
774	**Nonlinear Optical Measurement of the Local Berry Curvature in an atomically thin semiconductor**	Nele Tornow	Contributed talk (11:15-11:30)

Nele Tornow (1) Paul Herrmann (1) Clemens Schneider (2) Ferdinand Evers (2,3) Jan Wilhelm (2,3) Giancarlo Soavi (1,4)

(1) Institute of Solid State Physics, Friedrich Schiller University Jena, Jena, Germany
(2) Institute of Theoretical Physics and Regensburg Center for Ultrafast Nanoscopy, Regensburg, Germany
(3) Halle-Berlin-Regensburg Cluster of Excellence CCE, Regensburg, Germany
(4) Abbe Center of Photonics, Friedrich Schiller University Jena, Jena, Germany

With its direct relation to many exotic transport phenomena, quantum geometry is a fundamental concept in solid state physics. However, measurements of the local quantum geometry, e.g., Berry curvature, has been possible to date only via angle-resolved photoemission spectroscopy [1]. On the other hand, in one of our recent theoretical works [2] we have shown that there is a link between linear circular dichroism and derivatives of Berry curvature in 3D crystals with preserved time-reversal symmetry (TRS). In this presentation I will further demonstrate both, experimentally and with analytical solutions of semiconductor Bloch equations, that in a 2D semiconductor with broken TRS, the emerging second-harmonic circular dichroism can be used as a direct probe of the Berry curvature at the opposite K valleys in an atomically thin semiconductor, providing a new all-optical approach to access the local quantum geometry in 2D materials [3].

[1] Schüler, M. et al., Sci. Adv. 6, eaay2730 (2020)
[2] Soavi, G. and Wilhelm, J., arXiv:2501.03684 (2025)
[3] Tornow, N. et al. arXiv:2604.13729 (2026)

773	**Tracing THz-induced metastability and coherent collective modes in a layered quantum material at the angstrom scale**	Melanie Müller	Invited talk (11:30-12:00)

L.E. Parra López (1) J. Quan (2) A. Vaitsi (1) V. Sleziona (1) F. Schulz (3) A. Rubio (2) M. Wolf (1) Melanie Müller (1,4)

(1) Fritz Haber Institute of the Max Planck Society, Berlin, Germany
(2) Max Planck Institute for the Structure and Dynamics of Matter, Hamburg, Germany
(3) CIC nanoGUNE, Donostia-San Sebastian, Spain
(4) University of Bonn, Bonn, Germany

1T-TaS_2 is a layered quantum material hosting an insulating commensurate charge density wave (CDW) phase at low temperatures. The insulating nature of this phase arises from a complex interplay between electron-phonon coupling, electron-electron correlations and interlayer orbital hybridization, making it highly susceptible to external perturbations and atomic-scale disorder. In particular, it is known that ultrafast laser excitation, electrical pulses, or surface defects can drive 1T-TaS_2 into a metastable metallic mosaic phase at low temperatures. However, achieving a detailed understanding of how the nanoscopic environment influences the formation and ultrafast dynamics of such phases remains challenging. Terahertz-scanning tunneling microscopy (THz-STM) has emerged as a powerful technique for investigating nonequilibrium states with femtosecond-time and sub-nanometer spatial resolution [1,2]. Moreover, it has been shown recently that the tip-enhanced THz-fields can drive metastable phases via altering interlayer degrees of freedom in layered materials [3]. Here, we use THz-STM to investigate the local formation as well as the photoinduced dynamics of a THz-induced metastable state in 1T-TaS_2 [4]. We show that THz excitation drives the TaS_2 surface into a long-lived metastable state with a locally altered interlayer stacking order. In addition, by using optical-pump THz-probe measurements to probe its ultrafast response to optical excitation, we locally probe coherent oscillations of the local charge density, revealing the presence of multiple phonon modes including the intralayer CDW amplitude mode and two previously unreported interlayer shear and breathing modes. Our work establishes THz-STM as a powerful platform for imaging and controlling nonequilibrium quantum phases at their intrinsic spatiotemporal scales.

[1] M. Müller. Prog. Surf. Sci. 99, 100727 (2024)
[2] T. Cocker et al., Nature Phot. 15, 558–569 (2021)
[3] Jelic et al., Nature Phot. 19, 1048–1055 (2025)
[4] L. Parra López et al., arXiv:2505.20541 (2025)

205	**Dynamical Control of Coulomb Interactions and Hubbard Bands in Monolayer 1*T*-TaS_2**	Niklas Notter	Contributed talk (12:00-12:15)

Markus Aichhorn (1) Anna Galler (1) Niklas Notter (1)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

Monolayer 1T-TaS_2 hosts a star-of-David charge-density wave (CDW) that stabilizes a low-temperature Mott-insulating state. Recent time-resolved spectroscopies indicate a coupling between the CDW amplitude mode and the electronic correlation strength, yet the role of the screened Coulomb interaction remains unclear. Using the constrained random-phase approximation, we show that the CDW amplitude modifies the bare and screened on-site interactions, leading to sizable variations in the effective Hubbard U. Our combined density-functional and dynamical mean-field theory calculations reveal that the Hubbard bands shift in concert with the CDW amplitude and that a reduced distortion drives a transition from a Mott insulator to a correlated metal. These results demonstrate a direct link between lattice distortions and Coulomb interactions in transition-metal dichalcogenides, providing a microscopic mechanism for light-induced control of correlated phases in two-dimensional quantum materials.

M16 - Advances in Ultrafast Time-Resolved Ellipsometry

M16 – Session 1 (Tue 22. 10:30-12:30)			
ID	Title	Speaker	Type
691	**Challenges in Quantitative Analysis of Pump-Probe Ellipsometry Data**	Noah Stiehm	Invited talk (10:30-11:00)

Noah Stiehm (1) Huy Nguyen Vu (1) Jana de Wiljes (2) Stefan Krischok (1) Rüdiger Schmidt-Grund (1)

(1) TU Ilmenau, Technische Physik 1
(2) TU Ilmenau, Mathematics of Data Science

Pump-probe ellipsometry has the ability to capture many essential aspects of a material's excited states and their dynamics, e.g. relaxation, recombination and scattering rates, carrier temperatures, bandgap renormalization, and band-filling effects. Quantitative analyses of selected of these aspects are carried out in the community with increasing success. With access to electronic structure calculations it is also possible to form a reasonably comprehensive picture of charge carrier dynamics from observed transient ellipsometry spectra.
However, in trying to fit models in which the transient dielectric function is derived from underlying charge carrier dynamics, we regularly encounter challenges. These are on the one hand technicalities like parameter correlations and badly conditioned Hessians of the cost function or likelihood, but also seemingly more fundamental inconsistencies between the assumed models and the processes underlying the real measurement data, especially as occupations of excited states approach conditions of population inversion.
In this talk we present, based on pump-probe ellipsometry measurements of different semiconductors, doped glasses and metals, how these difficulties present themselves, and how we may tackle them with numerical techniques, additional information from other experiments, and careful treatment of artifacts arising from the use of short pulses.

764	**Photoinduced Ultrafast Phase Transition in VO2 Thin Films Monitored by Time-Resolved Spectroscopic Ellipsometry**	Mateusz Rebarz	Invited talk (11:00-11:30)

Mateusz Rebarz (1) Sébastien Cueff (2) Shirly Espinoza (1) Yael Gutiérrez (3) Krishna Khakurel (1) Shriram Ramanathan (4) José M. Saiz (3) Saul Vázquez-Miranda (1) Zhen Zhang (4)

(1) ELI Beamlines Facility, The Extreme Light Infrastructure ERIC
(2) Ecole Centrale de Lyon, CNRS, INSA, Université Claude Bernard Lyon 1
(3) Departamento de Física Aplicada, Universidad de Cantabria
(4) School of Materials Engineering, Purdue University

Phase-change materials (PCM) can undergo fast and reversible changes between crystalline and amorphous phases what makes them great candidates for many reconfigurable photonic devices. A thorough understanding of processes affecting local and temporal optical constants of PCMs provides the knowledge of technological limitations of these materials and their applicability. The changes in optical and electrical properties can be induced thermally, electrically or optically. Photoexcitation by laser pulses opens the perspective of monitoring even ultrashort changes in subpicosecond timescale. Employment of broadband ultrashort laser pulses for time-resolved ellipsometry enables monitoring ultrafast temporal evolution of the complex dielectric function of the studied material [1]. Here, we present application of this technique to study the ultrafast dynamics of the photoinduced insulator-to-metal transition (IMT) in vanadium dioxide (VO2) thin films [2]. We have identified distinct thermal and non-thermal dynamics in the photoinduced IMT, which critically depends on the exciting wavelength and fluence. Time evolution of the pseudodielectric function of the VO2 thin film during thermally and photoinduced phase transitions reveals that the primary differences in the IMT pathways are driven by nonequilibrium dynamics during the first picosecond after the photoexcitation. These and other findings of the study underscore the utility of time-resolved pump–probe spectroscopic ellipsometry as an effective tool for investigating phase transitions in strongly correlated materials.

[1] S. Richter et al. (2021), Rev. Sci. Instrum., 92, 033104.
[2] Y. Gutiérrez et al. (2024), ACS Photonics, 11, 4883-4893.

63	**Observation of entangled electron-zone boundary phonon states with transient spectroscopic ellipsometry**	Kurt Hingerl	Contributed talk (11:30-11:45)

Kurt Hingerl (1)

(1) Johannes Kepler Universität Linz

Silicon has three optical phonons, which remain inaccessible with linear optical techniques. Here we demonstrate that time-resolved pump-probe spectroscopic ellipsometry enables the detection of optical phonon responses at both the Brillouin zone center and -edge. Using pump pulses with photon energies below the indirect bandgap of silicon, we leverage two-photon absorption to induce sub-bandgap excitation. Transient optical effects have been probed in the 1.9-3.6 eV spectral range with pump-probe time delays from 50 fs to 4.5 ns. We observed distinct features indicating optical transitions involving entangled (coherent) electron phonon states:
1) a structure at the E1 critical point persisting for 4.5 ns;
2) longitudinal optical phonons with an energy spacing of 57±9 meV, lasting approximately 300 fs, and
3) two-phonon replicas, exhibiting a spacing of 81±7 meV.

Details of the presentation can be found in the main text and in the supplementary material of https://doi.org/10.1063/5.0288893.

481	**Transient Pump-Probe Ellipsometry on Organic and Inorganic Thin Films: Excitons versus Free Charge Carriers**	Manuela Schiek	Contributed talk (11:45-12:00)

Manuela Schiek (1,2)

(1) JKU Linz, Austria
(2) PTB Braunschweig, Germany

Using ultrafast spectroscopic ellipsometry, we aim to determine the transient dielectric function on a sub-picosecond timescale of organic and inorganic semiconducting thin films. We pick two thin film sample systems that differ in their electronic signature, namely bound excitons versus free Drude electrons: an organic semiconductor type consisting of solution-processed anilino squaraine dyes [1] and an inorganic transparent electrode consisting of sputter-coated indium tin oxide. [2] Transient pump-probe measurement techniques pose technical challenges when transferred to an ellipsometric setup [3] and place high demands on the samples.

[1] A. Minenkov, S. Hollweger, J. Duchoslav, O. Erdene-Ochir, M. Weise, E. Ermilova, A. Hertwig, M. Schiek. ACS Appl. Mater. Interfaces 16 (2024) 9517.
[2] R. Bernhardt, L. Rieland, T. Wang, M.F. Schumacher, A. Lützen, M. Schiek, P.H.M. Loosdrecht. Aggregate 6 (2025), e698.
[3] S. Richter, M. Rebarz, O. Herrfurth, S. Espinoza, R. Schmidt-Grund, J. Andreasson. Rev. Sci. Instrum. 92 (2021) 03104.

M17 - Emerging Trends in Dielectric Nanophotonics

M17 – Session 1 (Tue 22, 10:30-12:30)			
ID	Title	Speaker	Type
37	**Discovering new high-refractive-index optical materials**	Søren Raza	Invited talk (10:30-11:00)

Søren Raza (1)

(1) Technical University of Denmark

The discovery of new high-refractive-index dielectric materials is essential for advancing optical nanotechnologies, including metasurfaces, nanoantennas, and photonic devices operating across the visible and ultraviolet spectra [1]. While traditional materials like silicon and gallium phosphide have enabled much of the progress in all-dielectric nanophotonics, expanding the palette of high-index materials remains a key challenge, particularly for the ultraviolet and visible ranges.
In this talk, we present a combined theoretical and experimental approach to discovering new high-index materials. We first highlight our discovery of boron phosphide (BP), identified via high-throughput density functional theory (DFT) screening of over 2000 stable binary compounds [2]. BP offers a refractive index exceeding 3 with low absorption losses across the infrared to near-ultraviolet, a property validated experimentally through dark-field scattering and electron energy-loss spectroscopy of BP nanoparticles. These particles exhibit Mie resonances, demonstrating the potential of BP for optical applications in both the visible and near-ultraviolet spectral ranges.
Building on this methodology, we recently explored van der Waals materials and identified hafnium disulfide (HfS2) as a promising high-index candidate. Our ab initio calculations predict an in-plane refractive index above 3 with strong optical anisotropy in the visible range. Experimental ellipsometry confirms these predictions, and we further demonstrate the photonic potential of HfS2 by fabricating nanodisk resonators that exhibit Mie resonances in the visible spectrum. While we observe some chemical degradation of HfS2 when stored in ambient conditions, we show this can be mitigated by controlled storage environments.
Together, these studies showcase a pathway to discovering and experimentally validating new high-index materials, enabling future advances in nanoscale optics.

[1] S. Raza, K. S. Thygesen, and G. Naik, “Breaking the Moss rule”, arXiv:2602.16247 (2026).
[2] M. K. Svendsen, H. Sugimoto, A. Assadillayev, D. Shima, M. Fujii, K. S. Thygesen, and S. Raza, “Computational discovery and experimental demonstration of boron phosphide ultraviolet nanoresonators”, Adv. Optical Mater. 10, 2200422 (2022).
[3] X. Zambrana-Puyalto, M. K. Svendsen, A. H. Søndersted, A. Sarbajna, J. P. Sandberg, A. L. Riber, G. Ermolaev, T. M. Boland, G. Tselikov, V. S. Volkov, K. S. Thygesen, and S. Raza, "Computational discovery and experimental validation of of high-refractive index HfS2 nanoresonators", Sci. Adv. 11, eadw9339 (2025).

158	**Hybrid Dielectric Nanophotonics with 2D Semiconductors: Scalable Platforms for Valley-Selective Light–Matter Interactions**	Zlata Fedorova	Contributed talk (11:00-11:15)

Zlata Fedorova (1)

(1) Friedrich-Schiller-Universität Jena

Atomically thin transition metal dichalcogenides (TMDs) provide a unique excitonic platform for dielectric nanophotonics, combining strong light–matter interaction, pronounced nonlinearities, and internal valley degrees of freedom with inherent compatibility for planar integration. In this talk, we present recent advances in hybrid systems that integrate TMD monolayers with high-index dielectric nanostructures and metasurfaces, aiming at scalable architectures for enhanced and controllable optical functionalities. We discuss how Mie-type resonances and collective modes in dielectric platforms can be harnessed to tailor exciton emission, manipulate polarization and valley-selective responses. Particular emphasis is placed on fabrication strategies enabling deterministic and large-area integration, as well as on the role of coherence, carrier dynamics, and symmetry in governing hybrid light–matter interactions. These developments position TMD-based hybrid nanophotonic systems as a versatile route toward compact, tunable, and potentially quantum-enabled devices, bridging excitonic materials with next-generation dielectric metasurface technologies.

423	**Bridging quantum to Classical Optics with Feibelman Parameters: from TDDFT to Mesoscopic Maxwell Solvers for Plasmonics**	Lorenz Huber	Contributed talk (11:15-11:30)

Lorenz Huber (1) Javier Aizpurua (2) Antton Babaze (2) Ulrich Hohenester (1) Silkin Vyacheslav (2)

University of Graz, Insitute of Physics, Graz, Austria
University of the Basque Country- Spain, Donostia International Physics Center DIPC, Donostia, Spain

Plasmonics enables light confinement at the nanoscale, leading to strong field enhancements (1). When dealing with sharp particle features, gaps, or field variations on the nanometer scale, quantum surface effects become significant. Conventional Maxwell descriptions of these systems can lead to inaccurate results under such extreme situations.
Recently, it has been suggested to account for quantum surface effects through mesoscopic boundary conditions (2) that incorporate frequency-dependent dispersive and/or nonlocal Feibelman parameters (3, 4). The theoretical and numerical foundations of this mesoscopic approach have advanced significantly over the past decade (2,5,6), and proved to describe the important quantum effects with sufficient accuracy, in comparisons to results from supplementary time-dependent density functional theory simulations (4). However, the availability of accurate and nonlocal Feibelman parameters, particularly for plasmonic materials like gold and silver, and their dispersive behavior, remains limited.
In this work, we present a consistent methodology to derive dispersive Feibelman parameters for gold-dielectric interfaces, starting from either ab-initio time-dependent density functional theory (TDDFT) or computationally cheaper self-consistent hydrodynamic models (7). The extracted parameters are then translated into the mesoscopic regime through modified boundary conditions, enabling their use in real-space analytical and numerical Maxwell solvers. We demonstrate the power of this approach by combining macroscopic structural effects with microscopic quantum corrections. Specifically, we accurately model realistic plasmonic systems, like nanoantennas and nanoresonators, by placing nanoparticles on stratified dielectric media while directly accounting for interfacial quantum effects. This hybrid framework, merging theoretical rigor with precomputed quantum mechanical information, enables fast and accurate simulations of optical resonances, which would be computationally prohibitive using pure TDDFT methods. Our approach paves the way for the design and tuning of plasmonic resonances in applications ranging from two-particle dimers to sub-nanometer meta-surfaces, bridging the gap between quantum and classical optics for next-generation nanophotonic devices.

1. U. Hohenester, “Nano and Quantum Optics”, Springer Cham, Switzerland (2020).
2. Y. Yang, D. Zhu, W. Yan, A. Agarwal, M. Zheng, J. D. Joannopoulos, P. Lalanne, T. Christensen, K. K. Berggren, and M. Soljacic, “A general theoretical and experimental framework for nanoscale electromagnetism”, Nature 576, 248 (2019).
3. P. J. Feibelman, “Surface electromagnetic fields”, Prog. Surface Science. 12, 287 (1982).
4. A. Babaze, T. Neuman, R. Esteban, J. Aizpurura, and A. G. Borisov, “Dispersive surface-response formalism to address nonlocality in extreme plasmonic field confinement”, Nanophotonics 12, 3277 (2023).
5. L. Huber and U. Hohenester, “A computational Maxwell solver for nonlocal Feibelman parameters on plasmonics”, J. Phys. Chem. C 129, 5 (2025).
6. U. Hohenester and G. Unger, “Nanoscale electromagnetism with the boundary element method”, Phys. Rev. B 105, 075428 (2022).
7. G. Toscano, J. Straubel, A. Kwiatkowski, C. Rockstuhl, F. Evers, H. Xu, N. A. Mortensen and M. Wubs, “Resonance shifts and spill-out effects in self-consistent hydrodynamic nanoplasmonics”, Nature Communications 6, 7132 (2015)

684	**A Novel Chiroptical Spectroscopy Technique**	Jorge Olmos	Invited talk (11:30-12:00)

Jorge Olmos (1) Ivan Fernandez-Corbaton (2) Cristina Sanz-Fernández (MPC)

Universidad Autonoma de Madrid
Karlsruhe Institute of Technology (KIT)
Centro de Física de Materiales (CFM-MPC), San Sebastián

Chiral objects typically exhibit a different extinction for the two circular polarizations of light. Researchers often detect the chirality of objects by measuring this extinction difference employing Circular Dichroism (CD) spectroscopy. In this talk, we present a new spectroscopy technique for detecting the chirality of spherical objects based on measuring the Stokes parameters at any non-forward angle. The chirality measure we introduce effectively eliminates achiral background noise and is independent of both the object's concentration and the optical path length. Furthermore, we demonstrate that the technique is robust and verifiable in-situ by measuring the Stokes vector at two different non-forward angles of choice.

287	**Enhanced Molecular Chiral Response Driven by Crosstalking Quasi-Bound States in the Continuum**	Diana Shakirova	Contributed talk (12:00-12:15)

Diana Shakirova (1) Hatice Altug (2) Andrey Bogdanov (3,4) Adrià Canós Valero (1,5) Daniil Riabov (2) Thomas Weiss (1)

(1) Institute of Physics, University of Graz, and NAWI Graz, Graz, 8010, Austria
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(3) Qingdao Innovation and Development Center of Harbin Engineering University, Qingdao, 266500, China
(4) School of Physics and Engineering, ITMO University, St. Petersburg, 191002, Russia
(5) Institute of Telecommunications, Riga Technical University, Riga, 1048, Latvia

Identifying the handedness of chiral molecules is of fundamental importance in chemistry, biology,pharmacy, and medicine. In this work, we predict the chiroptical response of a dielectric metasurface engineered to amplify molecular circular dichroism (CD) using a general electromagnetic theory of chiral light-matter interaction in arbitrary resonators. The idea behind this theory is the ability to reconstruct the optical response (i.e., transmission, reflection and absorption) from a system via its resonant states. We derive a recipe to maximize a particular mechanism of chiral light-matter interaction, namely, the modal crosstalk, by supporting two nearly degenerate, high-quality-factor resonant states known as quasi-bound states in the continuum. Our theoretical and numerical analysis predicts a pronounced differential transmittance ΔT that exceeds the detection threshold of standard spectrometers. For the proposed metasurface, the differential transmittance approximately equals CD and can be measured in experiment directly. Moreover, we provide several strategies to decrease the computational time of numerical simulations without loss of physics.

305	**Topology-Driven Exciton-Polaritonic Flatbands in Anisotropic van der Waals Metasurface**	Alexander Antonov	Contributed talk (12:15-12:30)

Alexander Antonov (1) Maxim Gorkunov (2,3) Connor Heimig (1,4) Andreas Tittl (1,4) Thomas Weber (1)

(1) Ludwig-Maximilians-Universität München
(2) National Research Nuclear University ’MEPhI’, Moscow
(3) National University of Science and Technology, ‘MISIS’, Moscow
(4) Institute of Photonics, Hamburg University of Technology, Hamburg

We demonstrate how in-plane material anisotropy reshapes the topology of photonic quasi-bound states in the continuum (qBICs) in a metasurface, enabling control over the formation of extended far-field photonic and polaritonic flatbands [1].
Starting from an isotropic metasurface with rotational symmetry - ensuring double degeneracy of the qBIC - we show, within the resonant-state expansion (RSE) formalism, that in-plane anisotropy lifts this degeneracy, giving rise to two distinct linearly polarized resonances. Furthermore, symmetry breaking splits polarization singularities of integer topological charges into pairs of half-integer singularities (photonic Dirac points) in momentum space, connected by a flat photonic dispersion. This topological landscape reshaping is also captured within the RSE framework, which provides the conditions for the emergence of photonic Dirac points and flatbands. Next, by employing nonlinear RSE [2], we incorporate an excitonic resonance as a pole in the dielectric function and theoretically demonstrate two distinct regimes of directionally hybridized exciton–polariton flatbands.
Finally, using the intrinsically anisotropic van der Waals material ReS2 [3], we experimentally confirm the predicted anisotropy-induced photonic and polaritonic transformations, paving the way for topology-driven control of distinct light-matter interaction dispersion regimes.

[1] C. Heimig et al., arXiv:2509.01258, 2025;
[2] E. Muljarov et al., Phys. Rev. B 93, 075417, 2016;
[3] B. Munkhbat et al., ACS Photonics, 9, 7, 2398–2407, 2022.

M17 – Session 2 (Tue 22, 16:00-18:00)			
ID	Title	Speaker	Type
427	**Sub-diffractional dielectric structures using STED-inspired optical lithography**	Thomas Klar	Invited talk (16:00-16:30)

Georgii Gvindzhiliia (1) Anastasiia Mikhailenko (1) Manuel Jahn (1) Thomas Klar (1)

(1) Johannes Kepler Universität Linz

Stimulated emission depletion (STED) broke the diffraction limit of resolution in fluorescence microscopy and it has been proposed that STED should be equally applicable to spatially control chemical reactions at the nanometre scale.1 Meanwhile, this prediction has been experimentally realized using free radical polymerization of mostly (meth)acrylates.2-4 Using transient-state absorption depletion (TAD) rather than STED, three dimensional structures of 40 nm size in lateral and axial direction can be realized, which corresponds to 1/20 of the excitation wavelength.5
However, this concept was restricted to free radical polymerization for a long time. Only recently, it has been transferred to optical nanolithography comprising cationic or oxidative polymerizations. For instance, we found a photosensitizer/initiator couple with which STED-inspired writing of sub-100 nm wide epoxide lines became possible.6, 7 Currently, we are exploring ways to optically interfere with the radical cation or the ketyl radicals of photo-initiators in order to prevent polymerization in the outer rim of the optical point spread function.
Besides, we also managed to write subdiffractional lines of □-conjugated PEDOT (poly-3,4-ethylendioxythiophen), either by two photon, ultra-slow scanning or by applying TAD.8, 9 Besides, polypyrrole lines are also investigated. Such □-conjugated structures are particularly intriguing because they hold promise for sub-diffractional organic electronic devices.

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(9) Gvindzhiliia, G.; Angerer, C.; Schwaiger, C.; Sivun, D.; Jacak, J.; Hild, S.; Klar, T. A. Sub-diffraction multiphoton polymerization of PEDOT. submitted 2025.
We acknowledge financial support by the Austrian Science Fund (FWF) DOI: 10.55776/PAT3523723

300	**Pole expansion of the scattering matrix via rescaled scattering channels**	Elias Fösleitner	Contributed talk (16:30-16:45)

Elias Fösleitner (1) Adrià Canós Valero (1,2) Zoltan Sztranyovszky (3) Egor Muljarov (4) Kirill Koshelev (5) Thomas Weiss (1)

(1) Institute of Physics, University of Graz, and NAWI Graz, Graz, 8010, Austria
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(3) University of Birmingham
(4) Cardiff University
(5) Australian National University

The scattering matrix, which connects the incoming and outgoing waves of a scatterer, plays a central role in describing light-matter interaction and its pole expansion provides a powerful framework for replacing full-wave simulations with resonance-based models. In this work, we investigate the analytic continuation of the optical scattering matrix and its pole expansion in terms of optical resonances for spherical particles. While it is well established that resonance frequencies appear as poles of the scattering matrix in the complex frequency plane, obtaining a pole expansion using the Mittag-Leffler theorem remains challenging for the commonly used scattering channels from Mie theory, due to their exponential divergence in the complex frequency plane.
We demonstrate that a Mittag-Leffler expansion of the scattering matrix becomes possible through an appropriate rescaling of the basis, i.e., the incoming and outgoing waves, and provide a rigorous framework on how this rescaling of the basis affects the scattering matrix. We show that certain rescalings remove exponential divergences in the scattering matrix, which we refer to as regularization. Moreover, we demonstrate that the choice of rescaling is not unique and that certain choices can fundamentally alter the analytic continuation of the scattering matrix. We identify the emergence of additional, non-physical poles, referred to as channel poles, that do not originate from the optical resonances of the system.
These results suggest that regularizations of the scattering matrix can enable efficient pole expansion schemes for more complex three-dimensional scatterers, thereby broadening the range of systems accessible to modal analysis in photonics.

653	**Temporal dynamic scattering of resonant metastructures**	Kirill Koshelev	Invited talk (16:45-17:00 min.)

Kirill Koshelev (1) Hao Wu (2) Andrey Miroshnichenko (2)

(1) Department of Electronic Materials Engineering, Research School of Physics, Australian National University
(2) School of Engineering and Technology, University of New South Wales at Canberra

Scattering by dielectric resonant nanoparticles has been widely explored as a route to tailoring electromagnetic responses, yet most studies focus on steady-state behaviour. Here, we investigate the transient scattering response of Mie-resonant dielectric metastructures driven by short sub-picosecond pulses, extending resonant metaphotonics into the time domain.
We develop an analytical framework based on resonant state expansion of the time-dependent scattering Mie coefficients into exact contributions from the quasi-normal modes of the resonant structure, using recently established normalization, orthogonality, and completeness relations. The theory is validated against full-wave FDTD simulations in Ansys Optics and further applied to a CMOS-compatible metastructure design.

For a silicon sphere, we show that resonant excitation produces scattered-power dynamics dominated by a single quasi-normal mode, with exponential energy loading and release during the transient response. In contrast, in the anapole regime, sharp scattering bursts appear at pulse switch-on and switch-off due to energy trapping and release through a dynamic scattering dark state, analogous to metamaterial-induced transparency. These peaks arise from interference between a single quasi-normal mode and a broadband non-resonant background, and their temporal bandwidth is set by the quasi-normal-mode lifetime, making it much shorter than the driving pulse. Similar resonant and anapole dynamics are found in forward and backward radar scattering and are reproduced in a practical silicon cylinder on glass. These results reveal unconventional transient regimes in dielectric metastructures with potential applications in ultrafast photonics, pulse compression and shaping, and nanoparticle sorting.

159	**Completeness of eigenmodes and calculation of light scattering with the resonant-state expansion**	Zoltan Sztranyovszky	Contributed talk (17:00-17:15.)

Zoltan Sztranyovszky (1) Wolfgang Langbein (2) Egor Muljarov (2)

(1) University of Birmingham
(2) Cardiff University

We present an eigenmode based method to calculate the scattering-matrix and the optical cross-section of resonators. The eigenmodes of the system of interest are calculated via perturbation of an analytically solvable basis system using the resonant-state expansion (RSE). The eigenmodes form a complete set, and one can construct the Green's function as a Mittag-Leffler series. The scattering-matrix can be uniquely linked to the Green's function, and from it the cross-section can be found [2]. The non-resonant contribution to the scattering-matrix is fully taken into account via the Green's function, thus there is no need for further fitting or other approximations. This method eliminates the overlap integrals between the excitation and the mode fields used in other approaches, making it computationally highly efficient. For illustration, the cross-section of a dielectric sphere and a cylinder is calculated over a broad frequency range. The perturbed modes form a complete set inside the basis system, both inside and outside of the resonator [3]. The impact of this on the scattering calculation and on other applications is also discussed.

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169	**AAA rational approximation for nanophotonic resonance problems**	Felix Binkowski	Contributed talk (17:15-17:30)

Felix Binkowski (1) Fridtjof Betz (1) Sven Burger (1) Martin Hammerschmidt (2) Lin Zschiedrich (2)

(1) Zuse Institute Berlin
(2) JCMwave GmbH

We investigate numerical approaches based on AAA rational approximation [1, 2] for applications in nanophotonics. The AAA algorithm provides a powerful framework for constructing low-dimensional models of photonic systems by identifying and approximating dominant resonances [3], which are critical for understanding the electromagnetic response functions of the systems [4,5].
Resonances are characterized by the poles of the response functions, and often only a few are required to model the system's behavior within a given frequency range [4]. We demonstrate the effectiveness of rational approximation across three photonic systems: (i) We study a chiral metasurface, where resonance modes are computed and modal expansions are performed. This example emphasizes that using rational approximation can be computationally efficient with respect to the required number of sampling points [6]. (ii) A photonic crystal fiber is investigated, where the method yields relevant resonance modes while filtering out cladding and higher-order modes [7]. (iii) We study systems with scattering thresholds, where hidden resonances can be revealed through rational approximation [8].

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682	**All-Dielectric Metasurfaces for High-Efficiency Color Down-Conversion in Next-Generation RGB MicroLEDs**	Hadi Shamkhi	Contributed talk (17:30-17:45)

Hadi Shamkhi (1) Tung Ha Son (1) Arseniy Kuznetsov (1)

(1) Institute of Materials Research and Engineering (IMRE), Agency for Science, Technology and Research (A*STAR)

While color down-conversion (DC) is poised to replace costly pick-and-place assembly for mass-producing RGB microLED displays, it currently faces critical bottlenecks: inefficient color conversion and uncollimated emission, particularly as pixel dimensions shrink below 2 μm. Current industry workarounds, such as thick quantum dot (QD) plates or complex vertical stacking, introduce significant thermal, cost, and optical compromises. To overcome these limitations, we demonstrate the integration of an all-dielectric metasurface engineered to systematically amplify the absorption and conversion efficiency of QD color converters. By designing the metasurface to support highly localized resonant modes, we significantly enhance light-matter interactions within the active medium. Experimentally, this approach yields absorption increases of 1.96x and 1.65x for green and red emitting QDs, respectively. Consequently, overall color conversion efficiency improves by 24% (green) and 15% (red) compared to planar references. These findings establish resonant all-dielectric metasurfaces as a scalable, competitive solution to current DC bottlenecks.

M18 - Light-Driven Processes at Interfaces

M18 – Session 1 (Thu 24, 10:30-12:30, Chair: Moritz Eder)			
ID	Title	Speaker	Type
209	**Light-Driven Chemistry at Plasmonic Interfaces: an Atomistic Perspective**	Tommaso Giovannini	Invited talk (10:30-11:00)

Tommaso Giovannini (1)

(1) University of Rome Tor Vergata

The optical response of plasmonic nanostructures can be tuned by varying their shape, size, and chemical composition [1]. Peculiar phenomena arise when a molecular system is adsorbed on the surface of plasmonic materials, ranging from surface-enhanced spectroscopies to photocatalysis [2]. The accurate description of the optical properties of the plasmonic substrates is thus crucial for an understanding of the physical phenomena occurring at the plasmon resonance frequency. Here, we present an atomistic, yet classical, approach to predict the plasmon properties of nanostructures of complex shapes. The method is general enough to describe any plasmonic material, including noble metal nanoparticles (Ag and Au) [3] and metal alloys [4]. The approach is also coupled to a quantum mechanical (QM) description of the molecular system adsorbed on the nanostructure surface [5]. The resulting mixed QM/classical method is then extended to various spectral signals, from surface-enhanced Raman scattering to surface-enhanced fluorescence.
We show that our classical approach for plasmonics can correctly reproduce reference ab initio data [3], and experimental trends [3-4], and can be applied to large-scale nanoplasmonic simulations (more than 1 million atoms). By properly accounting for the atomistic discretization of matter, we can accurately describe the nanoplasmonics of systems dominated by quantum effects, such as subnanometer junctions [3,6], and geometrical defects, such as picocavities [7]. Finally, we discuss the current challenges in the prediction of the light-driven phenomena at plasmonic interfaces by means of atomistic approaches, ranging from surface-enhanced spectroscopies to photocatalysis.

[1] K. L. Kelly et al., J. Phys. Chem. B 2003, 107, 668.
[2] J. Langer et al. ACS Nano 2019, 14, 28.
[3] T. Giovannini et al., ACS Photonics 2022, 9, 3025.
[4] L. Nicoli et al. Front. Photon. 2023, 1199598.
[5] P. Lafiosca et al., J. Chem. Theory Comput., 2023, 19, 3616.
[6] T. Giovannini et al., Nanoscale, 2019, 11, 6004.
[7] T. Giovannini et al. Nano Lett. 2025, 25, 10802.

This work has received funding from the ERC under the European Union's Horizon Europe research and innovation programme (grant no. 101219149, project CHOPIN). Views and opinions expressed are however those of the author only and do not necessarily reflect those of the European Union or ERC Executive Agency. Neither the European Union nor the granting authority can be held responsible for them.

177	**Photocatalysis for Solar Fuels: Exploring interfaces in well-defined Hybrid Molecular Photosystems**	Stephen Nagaraju Myakala	Contributed talk (11:00-11:15)

Stephen Nagaraju Myakala (1) Jatin Chauhan (1) Alexey Cherevan (1) Dominik Eder (1) Sreejith P. Nandan (1) Carsten Streb (2) Samar Batool (1)

(1) Technical University of Vienna
(2) Johannes Gutenberg University Mainz

Due to the ongoing global warming and the upcoming energy crises, the exploitation of alternative, renewable energy sources has become a major focus of materials chemistry. The ultimate solution for sustainable energy lies in the concept of solar fuels – commodity chemicals that can be generated from nothing but sunlight and abundant feedstock through heterogeneous photocatalysis. The reactions of water splitting and carbon dioxide photoreduction, however, involve complex multi-electron redox processes that require a rational design of the surface catalytic sites. When working with ill-defined inorganic surfaces, these sites are inevitably hard to study and understand on a truly fundamental level, which limits the development of active and selective photocatalysts.
Homogeneous photocatalysis has developed largely independently from its heterogeneous counterpart and has achieved greater success in the rational design of organometallic photocatalysts, largely due to principles derived from coordination chemistry. Nevertheless, molecular photocatalysts encounter distinct limitations, including inadequate redox stability and the requirement for an additional molecular photosensitizer to facilitate light absorption.
In this talk, I will demonstrate that a rational integration of both photocatalytic approaches can address their respective limitations and contribute to bridging the gap between the two communities. As prime examples of this combination, we employ a diverse set fully-inorganic molecular clusters as surface-immobilized co-catalysts for photocatalytic water splitting reactions.[1-3] First, I will discuss covalent attachment of an anionic thiometalate cluster ([Mo3S13]2-) to the photoactive TiO2 surface for photocatalytic hydrogen evolution.[4] Second, I will present two exemplary POMs anchored onto TiO2 via linker-mediated electrostatic binding for photocatalysis.[5] In-depth characterization will unravel details of cluster immobilization, structural integrity and molecular nature of the attachment. Finally, photocatalytic experiments coupled with mechanistic studies will shed light on their stability, active sites, and long term performance.

[1] A. Cherevan et al., Advanced Science 2020, 7 (8), 1903511.
[2] S. Batool et al., Advanced Materials 2024, 36, 2305730
[3] ACS Nano 2026, 20, 1, 99–118
[4] S. Batool et al., ACS Catalysis 2022, 12, 6641–6650
[5] S. Nandan et al., ACS Materials Au 2022, 4, 505–515

723	**Nonequilibrium electron kinetics and interfacial charge transfer at plasmonically driven metal–molecule contacts**	Jon Scouten	Contributed talk (11:15-11:30)

Jon Scouten (1) Richard Gundermann (1) Evgenii Titov (1) Nicolas Jahn (1) Sergio Kogikosi (1) Namitha Deepak (1) Ilko Bald (1)

(1) of Potsdam

Light-driven charge transfer at metal–molecule interfaces depends on nonequilibrium electron dynamics in the nanoparticle and on the contact electronic structure. We present a model for a sulfur-linked molecule on a gold nanoparticle dimer, treating the nanoparticle as a geometry-aware metallic electron

system and the local Au–S–molecule region as a finite metal–molecule contact. A Maxwell–electron-hydrodynamic response gives the optical field, induced current, and density perturbation; these quantities drive a kinetic description of Fermi–Dirac and nonthermal electron populations, using plasmonic electron-generation models and energy-dependent e–e/e–ph scattering rates [1,3].
Interfacial fractional charge transfer is formulated by perturbing the coupling term in the reduced-density-matrix equation of motion [1,2]. The density perturbation and kinetic electron distribution estimate a fractional excess electron number η, defining an $N + \eta$ contact reference. The contact is treated as a density functional tight-binding (DFTB) subsystem coupled perturbatively to the nanoparticle-scale electron source. Linear-response time-dependent DFTB around this reference provides transition densities, orbital participation, and fragment charge redistribution across the Au–S–molecule interface [4].
The model determines how geometry-dependent nonequilibrium electron kinetics produces fractional interfacial charge transfer and molecular charge redistribution. It resolves charge-transfer channels by electron energy, hotspot localization, dimer geometry, and metal–molecule hybridization, and evaluates consistency with XPS binding-energy, valence-band, and work-function constraints [5].

558	**Near-Field Vibrational Energy Transfer and Upconversion in Plasmonic NanoCavities**	Rohit Chikkaraddy	Invited talk (11:30-12:00)

Rohit Chikkaraddy (1)

(1) University of Birmingham, UK

Near-field interactions provide a powerful route to mediate energy transfer between otherwise weakly coupled excitations. Here we demonstrate mid-infrared (MIR) donor–acceptor energy transfer and subsequent upconversion to visible emission enabled by ultrasmall plasmonic nanogap cavities [1,2]. The platform consists of metal–insulator–metal (MIM) resonators with gap sizes below 2 nm that producing extreme local density of optical states and strong light–matter coupling.
Within these cavities, molecular vibrations excited by continuous-wave MIR illumination act as energy donors. The tightly confined plasmonic near field couples these vibrational excitations to nearby electronic acceptors, enabling non-radiative vibrational–electronic energy transfer analogous to Förster-type processes but operating at vibrational frequencies. This mechanism circumvents the ultrafast vibrational relaxation that normally limits the observation of coherent vibrational energy flow in the MIR. The transferred energy is subsequently released as anti-Stokes visible emission, providing a direct optical readout of MIR excitation. Experiments reveal measurable upconversion efficiencies under low-power continuous-wave excitation, demonstrating that nanoscale optical confinement can bridge the large energy mismatch between MIR vibrations and visible electronic transitions. The results demonstrate a new regime of near-field mediated energy conversion where vibrational excitations act as donors in a plasmonically enhanced transfer process.
Beyond spectroscopy, this approach may enable room-temperature MIR detection, nanoscale sensing of molecular vibrations, and hybrid optomechanical platforms where molecular vibrations drive electronic or photonic responses.

A. Pal et al. Near-Field Vibrational Energy Transfer and Upconversion in Plasmonic Nanocavities. In review. (2026).
R. Chikkaraddy et al. Single-molecule mid-infrared spectroscopy and detection through vibrationally assisted luminescence. Nature Photonics* 17, 865-871 (2023).

602	**Disentangling electronic and phononic energy dissipation at non-contact junctions via first principles**	Lukas Hoermann	Contributed talk (12:00-12:15)

Lukas Hoermann (1) Reinhard Maurer (1,2)

(1) University of Vienna
(2) University of Göttingen

The vibrational dynamics of molecules in non-contact junctions depend critically on the geometric structure and electronic interactions between molecule and substrate. Vibrations excited by external stimuli dissipate energy into substrate electrons and phonons, affecting spectral linewidths, vibrational lifetimes, and the coupling between molecular and substrate phonons. We present a first-principles approach to disentangle the dissipation pathways by combining density functional theory, machine learning interatomic potentials (MLIPs), and non-adiabatic molecular dynamics. Using CO-functionalised Cu surfaces—prototypical systems for scanning probe and energy dissipation experiments—we train an MLIP that accurately captures molecule–substrate interactions. Electron-phonon coupling is incorporated via molecular dynamics with electronic friction. We reveal strong vibrational mode specificity sensitive to the tip–substrate geometry. Using equilibrium correlation function analysis, we extract phonon spectral functions and identify a weak non-additive effect where electron-phonon coupling enhances phonon-phonon relaxation. Our predicted vibrational lifetimes show good agreement with infrared and helium scattering experiments.

424	**Ultrafast photoinduced dynamics of hydrogen and functionalized thiolates on gold surfaces**	Shreya Sinha	Contributed talk (12:15-12:30)

Shreya Sinha (1) Peter Saalfrank (1)

(1) University of Potsdam

We investigate femtosecond laser induced, hot-electron mediated processes in hydrogen (atoms, molecules) and functionalized thiolates (S-CxHy) on gold surfaces (pristine, defected) via ab-initio molecular dynamics with electron friction treated under the Local Density Friction Approximation (LDFA). The time-dependent electronic temperatures in response to the laser pulse excitation are evaluated using the two-temperature model (2TM). Electronic vs. phononic dissipation effects across various laser pulse properties and initial surface temperatures are explored for the above processes. Additionally, charge transfer dynamics in the H2/Au(111) system is studied using a Gadzuk model type approach via constrained Density Functional Theory (DFT).

M18 – Session 2 (Thu 24, 16:00-18:00, Chair: Lukas Hoermann)			
ID	Title	Speaker	Type
553	**Light-induced structural dynamics: from static structure-property correlation of single metal nanoparticles to in situ TEM monitoring**	Wiebke Albrecht	Invited talk (16:00-16:30)

Wiebke Albrecht (1)

(1) AMOLF

Plasmonic nanoparticles can harness light and convert it into heat, charges, and localized electromagnetic fields, offering powerful pathways for sustainable chemistry. To unlock this potential, in my group we first establish quantitative correlations between nanoparticle structure and properties at the single-particle level, using advanced spectroscopic and electron microscopy workflows. In my talk, I will share key insights from these correlations and the workflows we developed. Building on these foundations, I will show how in situ TEM with light excitation allows us to directly monitor time-resolved atomic motion and structural dynamics, providing unprecedented insight into how light reshapes matter at the nanoscale. These insights not only deepen our fundamental understanding but also open routes to designing light-programmable catalysts and reactors with enhanced efficiency and selectivity.

750	**Model reactions in plasmon catalysis: from p-nitrothiophenol coupling to alkoxyamine homolysis**	Alina Gorbunova	Contributed talk (16:30-16:45)

Alina Gorbunova (1) Daria Votkina (2) Pavel Postnikov (2) Olga Guselnikova (1)

(1) Institute of Applied Physics, Vienna University of Technology
(2) Tomsk Polytechnic University

Transition to renewable energy is essential for sustainable development, with solar energy offering particularly promising route. Plasmon-active materials enable use of up to 70% of the solar spectrum in the visible and infrared ranges, providing low-energy alternative to UV-driven processes. Noble metal nanostructures (e.g. Au, Ag) exhibit localized surface plasmon resonance upon irradiation allowing efficient energy transfer to chemical systems and enabling reactions under mild conditions with high selectivity [1]. However, plasmon catalysis faces key challenges that hinder its industrial implementation among which the unclear reaction mechanism remains critical. In this pursuit, model reactions play central role. The most widely used system is the azo coupling of p-nitrothiophenol (PNTP) that leads to the formation of 4,4'-dimercaptoazobenzene (DMAB) under laser irradiation (Fig.1a). Despite its popularity with over 3000 published studies, its validity remains questionable.
In this work, we critically reassess the azo coupling as a model reaction for plasmon catalysis. Using X-ray photoelectron (XPS) and Raman spectroscopies, we demonstrate that plasmon excitation induces thiol desorption from Au nanoparticles via Au-S bond cleavage accompanied by thiol oxidation. Analysis of the N1s and S2p regions reveals a reaction pathway significantly more complex than commonly assumed (Fig.1b-d). This discrepancy highly impact on the plasmon catalysis mechanism conclusions made using azo coupling and show that PNTP azo coupling does not meet the criteria of reliable model reaction, namely simplicity and well-defined products. As an alternative, alkoxyamine homolysis can be used as a more suitable model reaction due to its well-established mechanism and straightforward kinetics. The adoption of appropriate model reactions is crucial for advancing mechanistic understanding and accelerating progress in plasmon catalysis.

1. S. Linic et al., Nat. Mater, 2015, 14, 567-576

672	**Heterogeneous Photocatalysis on Single-Crystalline Semiconductors**	Moritz Eder	Contributed talk (16:45-17:00)

Moritz Eder (1) Philip Petzoldt (2) Johannes U. Filzmoser (1) Jiri Pavelec (1) Martin Tschurl (2) Ulrich K. Heiz (2) Gareth S. Parkinson (1)

(1) TU Wien
(2) TUM

Light-driven chemistry at semiconductor surfaces couples photon absorption with thermal surface reactions in ways that are poorly understood at the molecular level. Using ultra-high vacuum (UHV) surface science techniques, we show how photocatalytic processes are composed of both thermal and photon-driven reaction steps, challenging the conventional "electrochemical" description of these systems.[1]
We present systematic studies of alcohol photocatalysis on well-defined TiO_2(110) single crystal surfaces, bare or decorated with metal clusters as co-catalyst. Alcohols can be converted into higher-value organic compounds and molecular H_2. Metal co-catalysts (Pt, Ni) do not merely act as electron sinks but actively participate in dark thermal chemistry, creating a synergistic mechanism where photogenerated carriers activate surface species and metal sites catalyze H_2 evolution. Furthermore, we quantitatively evaluate the mass spectrometric traces of the reactants, allowing us to quantify catalytic activity as well as reaction kinetics.[2][3]
Our results provide mechanistic understanding of heterogeneous photocatalysis, and extend the scope of chemical possibilities for selectively converting organic compounds. Key results can also be transferred to photocatalysis under ambient conditions.[4]

593	**Towards machine learning approaches in plasmonic solid–molecule systems for sensing and catalysis**	Olga Guselnikova	Invited talk (17:00-17:30)

Olga Guselnikova (1)

(1) Institute of Applied Physics, Vienna University of Technology

Plasmonic solid–molecule systems enable light-driven processes that couple electromagnetic field localization with interfacial energy transfer. However, the complexity arising from heterogeneous structures, dynamic interactions, and multiple coupled parameters limits quantitative understanding and predictive design. To quantitatively access and generalize these processes across plasmonic solid–molecule systems, machine learning (ML) methodologies are employed to probe dynamic processes and resolve chemical heterogeneity. These approaches were initially developed for surface-enhanced Raman spectroscopy sensing, enabling differentiation and quantitative analysis of multiplexed spectral signals in complex matrices. This is exemplified by the sensing of microplastics in wastewater and DNA fragments in biosamples. Building on this, ML is extended to catalytic systems with multiple coupled parameters (e.g., catalyst type, dosage, pH, etc.), where algorithms enable acceleration of catalytic discovery. Supported by high-throughput experimental platforms, this approach enables minimization of experimental effort while maximizing catalytic performance.

219	**Photoswitching of azobenzene derivatives on a Au(111) surface**	Matthew J. Timm	Contributed talk (17:30-17:45)

Matthew J. Timm (1) Robert di Vora (2) Haraprasad Mandal (1) Paul Schöngrundner (1) Stefan Hecht (3) Birgitta Bernhardt (2) Leonhard Grill (1)

(1) Institute of Chemistry, University of Graz, Austria
(2) Institute of Experimental Physics, Graz University of Technology, Austria
(3) Department of Chemistry & IRIS Adlershof, Humboldt-Universität zu Berlin, Germany

The light-induced trans-cis isomerization of azobenzene and its derivatives is of great scientific and technological interest as these molecule-sized photo-switches can be used for nano-scale sensing [1] or information storage [2]. Particularly, 3,3',5,5'-tetra-tert-butylazobenzene (mTBA) adsorbed on Au(111) has seen much interest, being studied at low coverages (< 0.1 ML) by scanning tunneling microscopy (STM) [3] and near monolayer coverage (0.9 ML) by two-photon photoemission [4]. However, missing is a single-molecule level insight into how photo-switching behaviour compares at different coverages. Here, we combine STM with a self-designed computer-vision algorithm to study photoisomerization induced by pulsed laser radiation at high surface coverage (0.6 ML to 0.9 ML). This approach can track the isomerization state of thousands of individual mTBA molecules and enables us to detect subtle variations in switching yields among densely packed, similarly oriented molecules. Further, at these high surface coverages we identify two packing phases that exhibit different photo-isomerization rates, over a variety of excitation wavelengths.

[1] V. Ferri, et al. Angew. Chem. Int. Ed., 47 (2008) 3407-3409.
[2] Z. F. Liu, K. Hashimoto, A. Fujishima. Nature, 347 (1990) 658-660.
[3] M. J. Comstock, et al. Phys. Rev. Lett. 99 (2007) 038301.
[4] S. Hagen, et al. Chem. Phys. Lett. 444 (2007) 85-90.

399	**How disorder impacts plasmonic and catalytic properties of (bi)metallic superlattices**	Adam Vavrečka	Contributed talk (17:45-18:00)

Adam Vavrečka (1) Juan Jesús Barrios Capuchino (2) Jonas Müller (1) Florian Schulz (3) Christian Schäfer (1)

(1) Institute of Applied Physics, TU Wien
(2) Universität Hamburg
(3) Universität Potsdam

Light–matter interactions constitute a promising route to tackle current energy challenges and reduce carbon footprint. For example, plasmonic materials, such as gold, copper, or aluminium, exhibit strong absorption in visible spectrum, offering an exquisite opportunity to utilize the sunlight in photocatalysis. [Linic et al., Nat. mater. 14 (2015)] It was shown that in closely packed bimetallic "antenna–reactor" configurations, they funnel incoming light into narrow regions near the reactor, which results in increased activity of the catalyst. [Herran et al., Nat. catal. 6 (2023)]
Using an exact, yet efficient mode-hybridization approach, we are able to go beyond the assumption of perfect surfaces and instead describe large disordered structures of (bi)metallic superlattices. This allows us to compare our predictions directly to experimental field maps obtained from Raman scattering (SERS). In particular, we study the effects of edges, terraces, or vacancies. Moreover, we investigate various configurations of bimetallic structures to maximize electric field enhancement, thereby achieving optimal catalytic efficiency. Our approach demonstrates that theory can pave the way towards better devices and sustainable chemical synthesis.

M18 – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
95 **P044**	**Photoisomerization of azobenzene derivatives on Au (111) using various photon energies and polarizations**	Haraprasad Mandal	Poster

Haraprasad Mandal (1) Paul Schöngrundner (1) Stefan Hecht (2) Leonhard Grill (1)

(1) University of Graz
(2) Humboldt-Universität zu Berlin

Azobenzene derivatives continue to serve as model systems for studying photoisomerization on surfaces. Among them, tetra-tert-butyl azobenzene (TBA) is particularly suitable, due to its chemical stability, large steric groups, and well-defined trans and cis configurations that can easily be identified in scanning tunnelling microscopy (STM) images.1,2,3 Using a tunable femtosecond laser and ultrahigh vacuum STM at low temperatures, we systematically investigated the photon-energy- and polarization-dependent trans-to-cis isomerization of TBA on Au(111). STM imaging was used to determine the configuration of individual molecules before and after laser exposure. The switching efficiency was studied for wavelengths between 350 nm and 800 nm and for different (s/p) polarization directions of the incident light. Our results provide insight into the parameters that steer TBA photoisomerization on Au(111) and demonstrate the capability of our laser–STM platform for controlled photochemical studies of single molecules.

264 **P045**	**Spectral signature of non-equilibrium, high-density incoherent excitons**	Katja Sophia Moos	Poster

Katja Sophia Moos (1) Juan Felipe Pulgarin Mosquera (1) Michael Schüler (1)

(1) Paul Scherrer Institut

The coherence of excitons, bound particle-hole pairs, is key for a number of non-equilibrium phenomena, including the amplification of ultrafast shift currents or "self-driven" exciton-Floquet effects. However, coherence is often suppressed by scattering processes on an ultrafast time scale. Still, such incoherent non-equilibrium states of excitons can have a profound impact on dynamical material properties. In this work, we investigate the effects of such long-lived non-equilibrium states for the single-particle spectral function and the signature in angle-resolved photoemission spectroscopy (ARPES). To this

end, we employ the non-equilibrium Green's function (NEGF) approach. To treat the excitons non-perturbatively, we use the particle-hole T-matrix. These calculations become tractable by using an efficient compressed representation in the exciton basis.

401 **P046**	**Machine-Learned Atomistic Simulations of Nonadiabatic Energy Transfer at Interfaces and Nanoclusters**	Fabian Jöbstl	Poster

Fabian Jöbstl (1)

(1) Universität Wien

Light-driven processes at surfaces and interfaces are governed by coupled electronic and atomic dynamics that strongly influence chemical reactivity under nonequilibrium conditions. Here, I investigate nonadiabatic energy transfer at surfaces, interfaces, and nanoclusters, with particular emphasis on how morphology and structural fluctuations affect reactivity. To access the relevant length and time scales, I develop and apply machine-learning interatomic potentials trained on first-principles data, enabling efficient simulations of structural dynamics and energy dissipation. These simulations are combined with mixed quantum-classical methods to describe nonadiabatic coupling between electronic excitations and nuclear motion beyond the Born-Oppenheimer approximation. This framework provides atomistic insight into excitation-induced energy transfer and allows for a systematic analysis of how light-induced structural changes in nanoclusters influence reaction pathways at surfaces and interfaces.

319 **P047**	**Vibrational Strong Coupling Modifies the Thermal Properties of Water**	Jonas Müller	Poster

Jonas Müller (1) Esmeé Berger (2) Paul Erhart (2) Eric Lindgreen (2) Christian Schäfer (1) Adam Vavrečka (1)

(1) Institute of Applied Physics, TU Wien
(2) Department of Physics, Chalmers University of Technology

In vibrational strong coupling, certain vibrational modes of molecules resonantly interact with the light modes confined by the cavity. The so-called polaritons formed by the strong interaction between light and matter share characteristics of both constituents, especially the non-local features of light. And indeed, experiments have highlighted that cavities can effect the energy transfer in molecular systems [Xiang et al., Science. 368.6491, 2020.].
In this talk, we present an in-depth investigation of the impact of strong coupling between a resonator mode with the vibrational modes of water. For this we employ machine-learning potentials combined with molecular dynamics to compare the dynamics of bulk water inside and outside of cavities. First results show faster redistribution of heat from hot vibrational modes into the bulk when coupled to a cavity compared to a system in free space.
At heart, this appears to originate from modified heat transfer under strong coupling and may provide insights into understanding clustering behavior under vibrational strong coupling [Dang et al., J. Phys. Chem. Lett. 16.47, 2025. Sandeep et al., Angew. Chem. Int. Ed. 138.1, 2026.].

595 **P048**	**Electronic friction simulations of laser-driven hydrogen evolution. Does surface coverage matter?**	Alexander Spears	Poster

Alexander Spears (1) Reinhard Maurer (1) Wojciech G. Stark (2)

(1) University of Vienna
(2) Imperial College London

Plasmonic catalysts such as metal nanoparticles harness the energy transfer between light, electrons and phonons at interfaces to drive chemical reactivity at interfaces. However, even on clean metal surfaces with a regular structure, it is unclear whether these dynamics are the result of mode-selective energy transfer or photothermal heating effects. Molecular dynamics simulations with electronic friction (MDEF) offer a quantum-classical description of electron-phonon coupling and have previously been used to model ultrafast dynamics on metal surfaces. Using machine learning surrogate models to accelerate MDEF simulations, we show that mode-selective energy transfer has a negligible influence on light-driven hydrogen evolution from copper surfaces at low coverages. We expect mode-selective energy transfer to play a stronger role at higher coverage, and show preliminary results for surface coverage dependence in laser-driven desorption from ruthenium as a function of different electronic friction approximations.

M19 - Time-Resolved Photoemission Orbital Tomography

M19 – Session 1 (Tue 22, 10:30-12:30)			
ID	Title	Speaker	Type
503	**Time-resolved Photoemission Orbital Tomography: The Route to Orbital Cinematography**	F. Stefan Tautz	Invited talk (10:30-11:00)

F. Stefan Tautz (1)

(1) Peter Grünberg Institute, Forschungszentrum Jülich, 52425 Jülich, Germany

During the last 15 years, a new variant of angle-resolved photoemission spectroscopy (ARPES) has been established: photoemission orbital tomography (POT). With POT, the wave functions of a molecule's individual electronic eigenstates (the orbitals) can be reconstructed in three-dimensional space, purely on the basis of experimental data. POT thus allows us to "observe the unobservable"---remember that unlike the probability density, the wave function itself is not a quantum mechanical observable in the strict sense.
Orbitals are important in chemistry because they form the basis of chemical bonding. They also come into play whenever light-matter interaction is involved, as in optoelectronics, light harvesting or lightwave electronics, since excited states can also be described in terms of orbitals. Therefore, observing the dynamics of orbitals on their intrinsic time scales can provide deep insights into the elementary mechanisms of many crucial processes in the natural sciences. This leads to the vision of an orbital cinematography. Time-resolved photoemission orbital tomography (trPOT) has the potential provide just this. Currently, a growing community of physicists and chemists is working towards this goal, and in this talk I will report some of the milestones that have been achieved. The talk will close with an outlook on future challenges and opportunities in the field of trPOT.

199	**Time-resolved photoemission orbital tomography of molecular excitations at surfaces**	Marcel Theilen	Contributed talk (11:00-11:15)

Marcel Theilen (1,2) Siegfried Kaidisch (3) Monja Stettner (4) Sarah Zajusch (2) Eric Fackelman (4) Alexa Adamkiewicz (2) Robert Wallauer (2) Andreas Windischbacher (3) Christian S. Kern (3) Michael G. Ramsey (3) Francois C. Bocquet (4) Serguei Soubatch (4) F. Stefan Tautz (4) Ulrich Höfer (1,2) Peter Puschnig (3)

(1) Universität Regensburg
(2) Philipps-Universität Marburg
(3) Universität Graz
(4) Forschungszentrum Jülich

Photoemission orbital tomography (POT) is a powerful technique, by which the electron distribution of orbitals of well-ordered molecules at solid surfaces can be imaged in momentum space [1]. Recently, we combined the method with laser pump-probe techniques to investigate the dynamics of charge transfer processes at molecular interfaces [2,3]. In this talk I will discuss how time-resolved POT (tr-POT) can image the momentum-space distribution and temporal evolution of molecular excitons [4]. These bound states of electrons and holes govern light-matter interactions in organic semiconductors, yet their full quantum mechanical wavefunctions have remained experimentally elusive.
For the model system α-sexithiophene (6T) on a Cu(110)-p(2x1)O surface, we determine a spatial extent of 9 Å for the exciton. It is seen to span about three neighboring molecules with a distinct phase modulation. From the temporal evolution of the recorded photoemission momentum maps, we derive a reduction of size of the exciton by about 25% during its 420-fs lifetime, which we attribute to self-trapping [4]. Our results resolve a long-standing debate on the exciton character in organic semiconductors and establish tr-POT as a general method to experimentally access exciton wavefunctions with spatial, phase and time resolution.

[1] P. Puschnig et al., Science, 326, 702 (2009)
[2] R. Wallauer et al., Science, 371, 1056 (2021)
[3] A. Adamkiewicz et al., J. Phys. Chem. C., 127, 20411 (2023)
[4] M. Theilen et al., arXiv:2511.23001 (2025)

475	**Capturing exciton wavefunctions by time-resolved photoemission orbital tomography**	Wiebke Bennecke	Invited talk (11:15-11:45)

Wiebke Bennecke (1)

(1) Georg-August-Universität Göttingen

Excitons are realizations of a correlated many-body wavefunction, consisting of a Coulomb-bound electron-hole pair. They are the dominant excitations in semiconducting organic and low-dimensional quantum materials and, thus, govern their optoelectronic response. To unlock the full optoelectronic potential and to control exciton-mediated energy conversion pathways, a microscopic understanding of excitons is crucial. Ultimately, this relies on access to the correlated exciton wavefunction, which has hardly been realized in experiments.
In this presentation, I will show how time-resolved photoemission orbital tomography can directly probe correlated exciton wavefunctions. I will demonstrate the power of this technique using the prototypical organic semiconductor C_{60} as an example, unraveling the exciton's multiorbital electron-hole contributions [1]. Building upon this, I will present our results on ultrafast exciton dynamics at the interface of the organic molecule PTCDA and monolayer WSe_2 [2]. Based on their unique momentum fingerprints, we can unambiguously identify the different excitonic states formed after optical excitation of WSe_2. Notably, our findings reveal a hybrid exciton state characterized by concomitant intra- and interlayer electron-hole transitions within the molecular layer and across the 2D-organic interface, respectively, which gives rise to an exciton wavefunction with a mixed Frenkel-Wannier character.
Finally, I will discuss our recent realization of a table-top three-dimensional photoemission orbital tomography scheme [3]. In this approach, we extend the photoemission momentum microscope with a spectrally tunable femtosecond high-harmonic generation (HHG) source and a tailored 3D reconstruction algorithm. This enabled us to image the frontier orbitals of PTCDA with full 3D resolution at strongly reduced experimental cost and paves the way for future time-resolved 3D wavefunction imaging.

[1] Bennecke, et al., Nat. Commun. 15, 1804 (2024)
[2] Bennecke, et al., Nat. Phys. 21, 1973–1980 (2025)
[3] Bennecke, et al., arXiv:2502.18269 (2025)

233	**Pushing subcycle momentum microscopy towards attosecond temporal resolution**	Jakob Helml	Contributed talk (11:45-12:00)

Jakob Helml (1) Manuel Meierhofer (1) Vincent Eggers (1) Lasse Münster (1) Giacomo Inzani (1) Leon Machtl (1) Suguru Ito (2) Changhua Bao (1) Robert Wallauer (2) Sarah Zajusch (2) Rimantas Budriūnas (3) Gerd Schönhense (4) Jens Güdde (2) Ulrich Höfer (1) Rupert Huber (1)

(1) Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN)
(2) Department of Physics, Philipps-Universität Marburg
(3) Light Conversion Ltd
(4) Institut für Physik, Johannes Gutenberg-Universität

Angle-resolved photoelectron spectroscopy with subcycle temporal resolution has emerged as a powerful technique for visualizing ultrafast carrier dynamics in the band structure of crystalline solids [1,2]. Yet, low probe photon energies limited these experiments to one-dimensional cuts through the center of the Brillouin zone. For orbital reconstruction via photoemission orbital tomography (POT), however, access to the entire two-dimensional momentum distribution is essential to capture all relevant signatures of molecular orbitals, which typically appear at large momentum values corresponding to the inverse of characteristic bond lengths [3].
Recently, we succeeded in combining phase-stable mid-infrared (MIR) pulses with MV/cm field strengths and an extreme-ultraviolet beamline generating few-femtosecond probe pulses. In combination with a time-of-flight momentum microscope, this enables the direct observation of strong-field effects on subcycle time scales across the entire first Brillouin zone of most quantum materials. The MIR field strength is even enough to directly alter inner molecular bonds and drive them on subcycle time scales. Additionally, a noncolinear optical-parametric amplifier provides wavelength-tunable excitation pulses. Therefore, the setup is also ideally suited to investigate phenomena like high-harmonic and high-order sideband generation, Floquet engineering, or Landau-Zener-Majorana transitions directly in the band structure [4].
In molecules, the energy differences between highest occupied (HOMO) and lowest unoccupied molecular orbital (LUMO) typically occur on the eV scale. A dedicated POT setup providing visible pump and isolated attosecond probe pulses at a repetition rate of up to 1 MHz may soon resolve the associated attosecond electron dynamics.

[1] Reimann et al., Nature 562, 396 (2018)
[2] Ito et al., Nature 616, 696 (2023)
[3] Wallauer et al., Science 371, 1056 (2021)
[4] Eggers et al., arXiv:2602.12844 (2026)

492	**Matrix element effects in time-resolved photoemission tomography from a non-equlibrium Greens function approach**	Christian Kern	Contributed talk (12:00-12:15)

Christian Kern (1) Davide Sangalli (2,3) Peter Puschnig (1)

(1) Institute of Physics, University of Graz
(2) Istituto di Struttura della Materia-CNR (ISM-CNR)
(3) European Theoretical Spectroscopy Facility (ETSF)

Non-equlibrium Greens function (NEGF) methods provide very powerful tools to simulate time-resolved photoemission spectroscopy [1], including the strong-field regime or experimental conditions where pump and probe pulses overlap in time. In the past, most applications of NEGF for tr-ARPES have concentrated on calculating the spectral function only, and have thus neglected effects of the probe pulse (or matrix-element effects). Especially for molecular systems, the latter can, however, be the dominant contributions to the photoemission signal and lie at the heart of photoemission (orbital) tomography (POT). In this contribution we show how a recently developed framework for matrix-element effects in exciton-POT [2] can be extended to NEGF methods, allowing for a simulation of pump-probe experiments in real-time.

[1] J. K. Freericks, H. R. Krishnamurthy and T. Pruschke, Theoretical Description of Time-Resolved Photoemission Spectroscopy: Application to Pump-Probe Experiments, PRL 102, 136401 (2009).
[2] S. Kaidisch, A. Kleiner, S. Refaely-Abramson, P. Puschnig and C. S. Kern, Photoemission tomography of excitons: momentum-space signatures of correlated electron-hole wave functions, arxiv.org/abs/2511.14956 (2026).

M19 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
245 **P017**	**Geometric and electronic properties of heptahelicene on Ag(110)**	Fabian Dixer	Poster

Fabian Dixer (1) Karl-Heinz Ernst (2) Christian S. Kern (1) Andrei C. Matetskii (3) Peter Puschnig (1) Serguei Soubatch (3) Frank Stefan Tautz (3)

(1) University of Graz
(2) Nanosurf Lab, Institute of Physics of the Czech Academy of Sciences, Czech Republic
(3) PGI-3, FZ Jülich and RWTH Aachen University, Germany

We present a density-functional theory (DFT) and time-dependent density-functional theory (TDDFT) investigation of the adsorption behaviour of heptahelicene (7HC) on Ag(110). This molecule serves as a model system for studying helical currents induced in chiral, spiral-like molecules on surfaces and has been discussed as an efficient spin filter due to the chirality-induced spin selectivity (CISS) effect. In our study, we first explore the adsorption energy landscape by sampling multiple initial configurations and performing local relaxations by using a repeated-slab approach with a van-der-Waals corrected GGA functional. The most favourable geometries are then examined in terms of work-function changes, charge-density-difference distributions, and projected densities of states. We further simulate photoemission momentum maps of the frontier molecular orbitals within photoemission orbital tomography and compare them with experimental angle-resolved photoemission data. This combined analysis provides a comprehensive understanding of the molecule–substrate interaction. It also forms the basis for future experimental studies of THz electric-field induced helical currents in the 7HC molecule. We simulate such transient currents by real-time, real-space TDDFT simulations for a gas phase heptahelicene molecule providing valuable insights into the induced charge rearrangements and currents.

265 **P018**	**Photoemission tomography of excitons in periodic systems**	Siegfried Kaidisch	Poster

Siegfried Kaidisch (1) Christian Simon Kern (1) Marcel Theilen (2) Monja Stettner (3) Eric Fackelman (3) Amir Kleiner (1) Sivan Refaely-Abramson (4) Frank Stefan Tautz (3,5) Ulrich Höfer (2,6) Peter Puschnig (1)

(1) University of Graz
(2) Universität Regensburg
(3) PGI-3, Research Center Jülich
(4) Weizmann Institute of Science
(5) RWTH Aachen, Germany
(6) Philipps-Universität Marburg

Photoemission orbital tomography (POT) is a combined experimental and theoretical technique that provides an intuitive understanding of angle-resolved photoemission spectroscopy (ARPES) in terms of electronic orbitals. The theoretical framework was recently extended to describe photoemission from excited states of gas-phase molecular systems [1], enabling theoretical insights into pump-probe ARPES experiments.
In this contribution, we present a further development toward photoemission from optically excited states in periodic systems. We derive a formula that allows for the computation of photoemission angular distributions based on GW/BSE results, discuss the approximations involved, and provide technical details of our implementation [2]. Finally, we demonstrate the capabilities of our approach on the example of an organic molecular layer (sexithiophene, [3]) and compare our predictions to corresponding time-resolved ARPES experiments. In particular, we show how the observed photoemission momentum pattern is related to the composition (BSE eigenvector) of the optically excited state and how information about the excited state's wavefunction may therefore be extracted from experimentally obtained momentum distributions.

[1] Kern et al., Phys. Rev. B 108, 085132 (2023)
[2] Kaidisch et al., arXiv: 2511.14956 (2025)
[3] Theilen et al., arXiv:2511.23001 (2025)

502 **P019**	**New laser system for time-resolved photoemission orbital tomography**	Eric Fackelman	Poster

Eric Fackelman (1) Francois C. Bocquet (1) Jens Güdde (2) Jakob Helml (3) Rupert Huber (3) Ulrich Höfer (3,4) Giacomo Inzani (1) Denis Krylov (1) Manuel Meierhofer (3) Lasse Münster (3) Peter Puschnig (5) Stefan Tautz (1) Robert Wallauer (4) Sarah Zajusch (4)

(1) Forschungszentrum Juelich GmbH
(2) Department of Physics, Philipps-Universität Marburg
(3) Department of Physics and Regensburg Center for Ultrafast Nanoscopy (RUN)
(4) Philipps-Universität Marburg
(5) University of Graz

We have built a 800 kHz high-power pump-probe femtosecond laser system for time-resolved photoemission orbital tomography experiments. It is designed to observe the excited-state orbitals of molecular monolayers adsorbed on a substrate. The pump leg uses commercial OPAs to generate excitation wavelengths from 325-450 nm and 630 - 900 nm with pulse energies around 1 µJ and includes a path for normal incidence pumping of the sample. For the probe beam, we use a commercial Multi-Pass Cell filled with Ar to compress the 1030 nm beam for frequency doubling and prism compression of the 515 nm as the fundamental for High Harmonic Generation, with a pulse energy greater than 30 µJ. Based on the setup in Marburg [1], we focus the 515 nm beam into an Ar jet delivered by a 30 um opening capillary, producing a strong 26.5 eV harmonic that enables access to a large momentum range for photoemission orbital tomography.

[1] Heyl, C. et al., J. Phys. B 45, 074020 (2012).

606 **P020**	**Molecular Orientation Determination of BTBT on Ag(110) Using Robust Sparse PhaseLift Orbital Tomography**	Kaori Niki	Poster

Kaori Niki (1) Shunnji Kamada (1) Ouki Watanabe (1) Masato Iwasawa (1) Yuri Hasegawa (1) Yoichi Yamada (1)

(1) Chiba University

Organic semiconductor thin films of 2,7-diphenyl-BTBT (DPh-BTBT) are known to exhibit high hole mobility, due to hybridization between the HOMO and HOMO−1 of neighboring molecules. Even the BTBT monolayer on Ag(111) with an asymmetric molecular arrangement can still retain enhanced transfer integrals and form dispersive bands [1]. In this study, we aimed to observe the fingerprint of the hybridization between the HOMO and HOMO−1 in the well-ordered monolayer of BTBT/Ag(110). However, the molecular orientation of each molecule remains unclear due to multiple domains. Puschnig has proposed the Orbital Tomography (OT) method, which reconstructs molecular orbitals from photoelectron momentum maps (PMMs) of molecules adsorbed on surfaces, and has elucidated adsorption structures [2]. We developed a Robust Sparse PhaseLift OT method to estimate molecular orbital coefficients from PMM data [3], which can be applied to reconstruct molecular orbitals from multi-domain monolayers.
In this presentation, PMMs of BTBT/Ag(110) were measured. By applying the Robust Sparse PhaseLift OT to this data, we estimate the molecular orbital coefficients to distinguish the molecular orientation of the multi-domain BTBT monolayer.
The PMM intensity can be expressed based on Fermi's golden rule as $I = \Delta^2 (a \cdot c)^2$, where Δ, a, and "c" denote the electron-photon interaction, atomic orbital Fourier transform, and molecular orbital coefficients. I is a squared quantity, the phase information is lost. In the Robust Sparse PhaseLift OT method, c is lifted to a matrix C to formulate a semidefinite program (SDP) with sparsity constraints. The estimated molecular orbital for configuration A agrees with DFT results, indicating adsorption on Ag(110).

[1] Y. Ono et al., Nanoscale, 17, 21729–21736 (2025).
[2] P. Puschnig et al., Science, 326(5953), 702-706 (2009).
[3] K. Niki et al., J. Phys. Chem. A, 128, 2672−2679 (2024).

M20 - The New Frontiers of Angle-Resolved Photoemission Spectroscopy: Spin, Time and Spatial Resolution

M20 – Session 1 (Mon 21, 16:00-18:00, Chair: Francesco Presel)			
ID	Title	Speaker	Type
395	**Single domain spectroscopic signatures of a magnetic Kagome metal**	Lukasz Plucinski	Invited talk (16:00-16:30)

Lukasz Plucinski (1)

(1) Forschungszentrum Juelich GmbH, Juelich, Germany

Spin- and orbital-resolved access to the electronic bands is necessary to establish key properties of quantum materials such as the quantum-geometric tensor. Despite the recent revival of interest in magnetic Kagome compounds, no spectroscopic access to their magnetic properties has been available so far due to small domain sizes and the lack of appropriate techniques. Furthermore, their real-space magnetic texture is often complex and temperature-dependent.
We investigate the magnetic Kagome metal $DyMn_6Sn_6$ using high-resolution micro-focused circular-dichroic angle-resolved photoemission (μ-CD-ARPES) to probe its magnetic and electronic properties. By tuning the kinetic energy to various features of the Dy $4f$ multiplet, we resolve magnetic domains in samples cryo-cooled down to 20 K. Smaller, but clear, signatures are also detected in the Mn $3p$ levels. The behavior of both Dy $4f$ and Mn $3p$ features is in remarkable agreement with our modeling based on the Hartree–Fock method, revealing ferrimagnetic alignment of Dy and Mn local moments and further strengthening our interpretation. Adjusting the energy to the Mn $3p$-dominated valence bands reveals signatures that we relate to the orbital magnetization through comparison with ab initio electronic structure calculations. Our study establishes spectroscopic access to a single magnetic domain in a Kagome metal and demonstrates μ-CD-ARPES as a direct probe of magnetic domain properties, opening the way for spatially resolved studies of complex magnetic phases in quantum materials.

arXiv:2507.12085 (2025); accepted for publication in Nature Communications.

740	**Momentum space signatures of molecular orbitals on a ferromagnetic surface**	Martin Anstett	Contributed talk (16:30-16:45)

Martin Anstett (1) Lu Lyu (2) Gyula Halasi (3) Csaba Vass (3) Nikolett Oláh (3) Martin Aeschlimann (1) Benjamin Stadtmüller (2)

(1) RPTU Kaiserslautern-Landau
(2) University of Augsburg
(3) ELI-ALPS Hungary

The integration of organic molecules with ferromagnetic surfaces is a promising approach to advance spintronic applications. Organic molecules provide tuneable electronic and spin-related properties, such as weak spin-orbit coupling and long spin coherence times. The ferromagnetic substrate provides the spin-polarized states necessary for spin injection and detection. The interaction between molecular orbitals and the ferromagnetic substrate plays a crucial role in controlling the spin-dependent transport and magnetic coupling at the interface.
This work focuses on the visualization of molecular orbitals on ferromagnetic surfaces at room temperature. The difficulty here is the lack of ordered or aligned molecular films on magnetic substrates to resolve molecular orbitals with ARPES. By depositing ultrathin cobalt films on Au(111) as a ferromagnetic platform, we achieve the formation of extended, self-assembled molecular structures. Using these molecular structures, we can combine spin- and momentum-resolved photoemission spectroscopy with photoemission orbital tomography to study the orbitals of the adsorbed molecules. Our analysis reveals how the molecules arrange on the cobalt surface, producing distinct photoemission signatures associated with individual molecular orbitals.

742	**Probing Spin-Dependent Electronic Structure Across an Oxide Barrier: Spin-Resolved ARPES of Buried MgO/Fe Interfaces**	David Janas	Contributed talk (16:45-17:00)

David Janas (1) Mira Arndt (1) Lasse Sternemann (1) Vitaliy Feyer (2,3) Iulia Cojocariu (4,5) Daniel Baranowski (2) Alessandro Sala (6) Andreas Windischbacher (7) Peter Puschnig (7) Stefano Ponzoni (8) Giovanni Zamborlini (7) Mirko Cinchetti (1)

(1) Department of Physics, TU Dortmund University
(2) PGI-6, FZ Jülich
(3) Universität Duisburg-Essen
(4) Physics Department, University of Trieste, 34127 Trieste, Italy
(5) Elettra – Sincrotrone Trieste S.C.p.A, 34149 Trieste, Italy
(6) CNR - Istituto Officina dei Materiali (IOM)
(7) Institute of Physics, University of Graz, 8010 Graz, Austria
(8) Ecole Polytechnique, CNRS, Institut Polytechnique de Paris

The spin-dependent electronic structure of buried oxide–ferromagnet interfaces governs the performance of magnetic tunnel junctions,[1,2] but remains difficult to access directly with conventional surface-sensitive spectroscopies. Here, we show that spin-resolved momentum microscopy, i.e. spin-resolved ARPES in full-field momentum-imaging mode, can probe the buried MgO/Fe(100) interface and reveal how atomic-scale oxygen control modifies spin-selective tunneling states.[3]
Using reactive MgO growth on Fe(100), we tune the interface from an oxygen-free termination to a fully oxygen-intercalated layer while preserving epitaxial order. Despite the insulating MgO overlayer, momentum-resolved photoemission detects pronounced interface-derived fingerprints in k-space that persist up to MgO thicknesses of 8 monolayers. These fingerprints provide a direct spectroscopic readout of the buried interface chemistry and allow us to distinguish oxygen-free, partially oxidized, and oxygen-intercalated terminations.
Most importantly, spin-resolved Fermi-surface maps reveal a strong dependence of the interfacial spin texture on oxygen incorporation. Spin-resolved Fermi-surface maps show that oxygen-free MgO/Fe interfaces strongly suppress minority-spin spectral weight at the Fermi energy, consistent with coherent spin filtering through crystalline MgO. In contrast, oxygen intercalation restores minority-spin intensity and reduces the spin contrast at the Fermi level. These results demonstrate that spin-resolved ARPES can directly access buried spintronic interfaces and visualize the electronic states underlying spin-selective tunneling. More broadly, they establish interfacial oxygen as a measurable and tunable parameter for engineering oxide–ferromagnet junctions.

[1] W. H. Butler et al., Phys. Rev. B 63, 054416 (2001).
[2] S. S. P. Parkin et al., Nat. Mater. 3, 862–867 (2004).
[3] D. M. Janas et al., Advanced Science, 2026, e23165.

699	**Unconventional magnetism**	Federico Mazzola	Invited talk (17:00-17:30)

Federico Mazzola (1)

(1) University of Padova

For many years, since the beginning of the 19th century, the existence of magnetism in low dimen-sions has been both desired and controversial. It was long thought, that magnetic orders in low di-mensional systems could not be realized at temperatures different from zero. At least, this was what the Mermin-Wagner theorem stated for isolated Heisenberg spins. The scarcity of low-dimensional materials with magnetic properties, and the partial understanding of the role of spin-anisotropy have supported this picture for several decades. In three-dimensions, magnetism has revolutionized our everyday life, enabling familiar technologies which are of common use. A few examples include com-puters' memories, RAM, hard-disks, key cards, credit cards, electric batteries, light, and distance sen-sors. This relentless pace of development has motivated the search for magnetism in systems with increasingly smaller sizes.
With cooperation of experimental and theoretical physics, researchers discovered that spin-anisotropy can stabilize low-dimensional magnetism. In this, spin-orbit coupling plays an important role. Surface experimental probes, such as angle-resolved photoelectron spectroscopy provide researchers access to the electronic structure of solids. Despite the advances in the field, recently, new forms of surface lo-cal magnetism completely different from standard descriptions have appeared, with relevance in quan-tum transport information, dissipationless transport, and quantum sensing.
Here, I aim to give an overview of a new powerful methodology to uncover hidden phases of elec-trons, including spins, and magnetism which was so fare elusive, and that we were able to uncover for the first time.

Nature 626, 752–758 (2024)
Nature Physics 19, 1135–1142 (2023)
Nature Physics 20, 1103–1109 (2024)
Nature Physics 21, 110–117 (2025)
Nature Communications 16, 4495 (2025)
Physical Review Letters 134, 066501 (2025)

627	**Spin polarization dynamics of free carriers in 2H-WSe_2**	Pierre Nonnon	Contributed talk (17:30-17:45)

Pierre Nonnon (1) Sourour Ayari (2) Daniel Ortiz Espinoza (1) Aki Ismo Olavi Pulkkinen (2) Habib Rostami (3) Emmanuele Cappelluti (4) Olivier Heckmann (1) Karol Hricovini (1) Jan Minar (2) Thierry Ruchon (5) Maria-Christine Richter (1) Romain Géneaux (5) David Bresteau (5) Mauro Fanciulli (1)

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We present Spin, Time-, and Angle-Resolved Photoemission Spectroscopy (STARPES) measurements of photoexcited free carriers in centrosymmetric bulk 2H-WSe_2. This setup combines a high harmonic generation (HHG) source with tunable repetition rate, pulse duration, photon energy, and polarization, and a hemispherical analyzer with a 3D VLEED spin detector.
The electron spin polarization dynamics in photoexcited 2H-WSe2 have been studied in different regimes. In the excitonic case[1], resonant pumping near the K-valley optical bandgap with a fluence below the critical Mott density creates bound excitons. Strong spin-integrated circular dichroism is then reported, along with valley and helicity dependence of the bright excitons' (K, K') spin polarization decaying within 100fs. In contrast, the momentum-forbidden dark exciton (electrons scattered into the Σ valleys) exhibits a time- and helicity-independent spin polarization, acting as a momentum-space spin-reservoir. At higher fluence[2], the system breaks into an electron-hole plasma, where Σ-valley spin polarization becomes valley- and helicity-dependent. Additionally, a spin polarization flip at longer timescales is observed for a single pump helicity, attributed to the intrinsic conduction band spin polarization. Both regimes yield distinct spin polarization behaviors, yet remain constrained by optical selection rules imposed by resonant pumping.
Here, we study the free carrier regime, accessed by pumping well above resonance with a 2.4eV, 350fs pulse. We observe free carriers in K and Σ valleys, finding a decay time at K of an order of magnitude slower than in the resonant case, comparable to that at Σ. Due to the large number of allowed transitions, scattering processes and spin polarization dynamics are expected to be significantly more complex than in the resonant case.
At time zero, the K and Σ spin polarization sign and magnitude are valley dependent but helicity independent. Furthermore, no spin polarization reversal is observed at longer timescales either at K or Σ. These results differ from both the excitonic and electron-hole plasma resonant regimes, providing a better insight into the complex spin dynamics in 2H-WSe_2.

[1] Fanciulli et al., Phys. Rev. Lett. 131(6), 066402 (2023)
[2] Hedwig et al., Phys. Rev. Lett. 135(18), 186903 (2025)

373	**ARPES simulations from first principles via Kohn-Sham scattering states**	Gian Parusa	Contributed talk (17:45-18:00)

Gian Parusa (1) Sotirios Fragkos (2) Samuel Beaulieu (2) Michael Schüler (1)

(1) Paul Scherrer Institute
(2) Universite de Bordeaux

Angle-resolved photoemission spectroscopy (ARPES) is a powerful probe of electronic structure, where the measured intensity is governed by the product of the single-particle spectral function and the photoemission matrix element. While the spectral function encodes intrinsic many-body electronic properties, the matrix element introduces strong modulations as a function of photon energy, polarization, and experimental geometry, which can complicate the interpretation of ARPES spectra. On the other hand, it carries valuable information about the quantum geometry of the electronic states, including orbital angular momentum and Berry curvature, which are central to topological phenomena and emerging orbitronic functionalities. These consideration highlight the need for accurate and efficient simulations of photoemission matrix elements, with particular emphasis on the treatment of photoelectron final states.

In this work, we model the photoelectron final state as a solution of the Kohn-Sham scattering problem in an ARPES geometry, subject to time-reversed low-energy electron diffraction (trLEED) boundary conditions. We benchmark our approach against experimental datasets of circular dichroism in ARPES across multiple photon energies and demonstrate the remarkable agreement. Our method establishes a practical and accurate framework for incorporating matrix element effects in ARPES simulations, enabling more reliable extraction of intrinsic electronic and topological properties as well as paving the way to ab initio description of pump-probe time-resolved ARPES.

M20 – Session 2 (Tue 22, 16:00-18:00, Chair: Giovanni Zamborlini)			
ID	Title	Speaker	Type
534	**Competing interactions in the electronic structure of advanced materials**	Claudia Draxl	Invited talk (16:00-16:30)

Claudia Draxl (1)

(1) HU Berlin

Many-body perturbation theory allows us to describe on the same footing the interplay between competing interactions of similar strength and on the same energy scale, which can give rise to exciting phenomena. In this talk, I will highlight the role of electron-electron interaction, electron-vibrational coupling, and electron-hole correlation to understand electronic excitations in different material classes. I will also discuss the need for the development of advanced methodologies to keep up with the rapid progress in experimental techniques like angle-resolved photoemission experiments. Recent examples [1-3] will comprise 2D materials as well as their interfaces with organic semiconductors.

[1] I. Gonzalez Oliva, S. Tillack, F. Caruso, P. Pavone, and C. Draxl, Impact of electron-phonon interaction on the electronic structure of interfaces between organic molecules and a MoS_2 monolayer. J. Chem. Phys. 164, 074704 (2026).
[2] W. Bennecke, I. Gonzalez Oliva, J. P. Bange, P. Werner, D. Schmitt, M. Merboldt, A. M. Seiler, K. Watanabe, T. Taniguchi, D. Steil, R. T. Weitz, P. Puschnig, C. Draxl, G. S. M. Jansen, M. Reutzel, and S. Mathias Hybrid Frenkel-Wannier excitons facilitate ultrafast energy transfer at a 2D-organic interface. Nat. Phys. 21, 1973 (2025).
[3] M. Schebek, I. Gonzalez Oliva, and C. Draxl, Efficient GW and BSE calculations of heterostructures within an all-electron framework. Phys. Rev. B 112, 165130 (2025).

163	**Circular dichroism in the photoelectron angular distribution of achiral molecules**	Peter Puschnig	Contributed talk (16:30-16:45)

Christian Simon Kern (1) Xiaosheng Yang (2,3) Giovanni Zamborlini (1) Simone Marini (4,5) Matteo Jugovac (4,5) Vitaliy Feyer (4,5) Umberto De Giovannini (6) Angel Rubio (6) Serguei Soubatch (2,3) Michael G. Ramsey (1) Frank Stefan Tautz (2,3) Peter Puschnig (1)

(1) University of Graz
(2) PGI-3, FZ Jülich
(3) RWTH Aachen, Germany
(4) PGI-6, FZ Jülich
(5) Universität Duisburg-Essen
(6) MPI for the Structure and Dynamics of Matter, Hamburg

Circular dichroism in the angular distribution (CDAD) is the effect that the angular intensity distribution of photoemitted electrons depends on the handedness of the incident circularly polarized light. CDAD has been reported also for achiral organic molecules at the interface to metallic substrates. For this latter case, we investigate two prototypical pi-conjugated molecules, namely tetracene and pentacene, whose frontier orbitals have a similar shape but exhibit distinctly different symmetries. By comparing experimental CDAD momentum maps with simulations within time-dependent density functional theory, we show how the final state of the photoelectron must be regarded as the source of the CDAD in such otherwise achiral systems. We gain additional insight into the mechanism by employing a simple scattering model for the final state, which allows us to decompose the CDAD signal into partial wave contributions.

266	**Tracing the film structure of an organic semiconductor with photoemission orbital tomography**	Monja Stettner	Contributed talk (16:45-17:00)

Monja Stettner (1) Siegfried Kaidisch (2) Andrey V. Matetskiy (1) Eric Fackelman (1) Serguei Soubatch (1) Christian Kumpf (1) François C. Bocquet (1) Michael G. Ramsey (2) Peter Puschnig (2) F. Stefan Tautz (1)

(1) PGI-3, Research Center Jülich
(2) University of Graz

Using angle-resolved photoemission spectroscopy, in particular photoemission orbital tomography (POT), we investigate the coverage-dependent electronic and geometric properties of the organic oligomer α-sexithiophene (6T) on Cu(110)-p(2×1)O [1]. The oxygen-induced reconstruction of the copper surface electronically decouples the molecules from the substrate [2]. By combining momentum-resolved experimental data with density functional theory calculations, we trace the transition of the film structure from a substrate-templated monolayer to bulk-like multilayers in a quantitative manner. Specifically, the tilt of the 6T molecules decreases from 37° (2 ML) to 31° (8 ML). The former is consistent with DFT and is governed by the oxygen row spacing, while the latter matches the structure of bulk 6T.
A previous study of this system [3] succeeded in disentangling effects of intra- and intermolecular delocalization and dispersion. To this end, band maps were measured either along or perpendicular to the long molecular axis. In our case, using photoemission momentum microscopy, we gained access to the 2D momentum space, enabling a significantly more comprehensive characterization. In particular, we identify an electronic band that exhibits clear intermolecular-dispersion character in one direction, while in the perpendicular direction electronic states remain confined at the molecular scale, revealing typical intramolecular dispersion. This suggests that, for certain states, electron delocalization within a molecule is comparable to that between molecules, marking the limit of a purely local orbital picture. This also implies that in optically excited states, excitons will likely extend over several adjacent molecules, which has recently been observed in a dedicated time-resolved POT study [4].

[1] Stettner et al., arXiv: 2603.06204 (2026)
[2] Yang et al., Chem. Commun. 54 (2018)
[3] Berkebile et al., Appl. Phys. A 95 (2009)

[4] Theilen et al., arXiv:2511.23001 (2025)

412	**Disrupting pi-Conjugation: How Carbonyl Groups Reshape the Electronic Landscape of Pentacene**	Andrei Matetskii	Contributed talk (17:00-17:15)

Francois C. Bocquet (1) Jonas Brandhoff (2) Roman Forker (2) Torsten Fritz (2) Elise Furch (2) Andrei Matetskii (1) Felix Otto (F2) Peter Puschnig (3) Michael G. Ramsey (3) Maximilian Schaal (2) Serguei Soubatch (1) F. Stefan Tautz (1)

PGI-3, Forschungszentrum Jülich
Friedrich Schiller University Jena
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π conjugation – the delocalization of electrons across a network of overlapping p orbitals is a foundational concept in organic chemistry, governing molecular stability, reactivity, and functionality across biological and technological domains. Aromaticity arises as a manifestation of this delocalization, where the population of delocalized bonding and antibonding orbitals, in accordance with Hückel's rule, imparts thermodynamic stability and chemical resilience. Disruptions to π conjugation – through steric twisting, oxidation, or structural distortion – diminish electron delocalization and promote the emergence of localized aromaticity, thereby drastically altering chemical reactivity and stability. Polycyclic aromatic hydrocarbons (PAHs) offer an ideal playground for investigating such effects, as they often tend to self-assemble on surfaces, enabling experimental study using conventional methods of surface science, e.g., low-energy electron diffraction and scanning tunneling microscopy. Photoemission orbital tomography (POT) [1] provides direct experimental access to the frontier orbital structure of PAHs [2] and reveals the nature of their aromaticity [3]. In this study, combining POT with conventional surface-science techniques and density functional theory (DFT) calculations, we show that keto-functionalization of a pentacene ($C_{22}H_{14}$) dramatically disrupts its π conjugation. The resulting 6,13-pentacenequinone ($C_{22}H_{12}O_2$) exhibits an orbital structure reminiscent of naphthalene ($C_{10}H_8$). This effect is attributed to a delocalization barrier for π electrons introduced by the keto groups at the molecule's core, effectively partitioning the molecule into two naphthalene-like segments with localized conjugation. As a consequence, we observe a notable increase in the energy gap between the highest occupied and lowest unoccupied molecular orbitals.

[1] Puschnig et al., Science 326 (2009) 702–706
[2] Lüftner et al., PNAS 111 (2014) 605–610
[3] Haags et al., ACS Nano 14 (2020) 15766–15775

59	**Momentum-resolved signatures of ultrafast orbital excitations in van der Waals antiferromagnets**	Mirko Cinchetti	Invited talk (17:15-17:45)

Mirko Cinchetti (1)

(1) TU Dortmund University

Angle-resolved photoemission spectroscopy (ARPES) has evolved into a powerful platform for probing not only the equilibrium electronic structure but also the ultrafast dynamics of correlated quantum materials. In this talk, I will highlight how time-resolved momentum microscopy based on high-repetition-rate fs-XUV sources enables full–Brillouin-zone mapping of nonequilibrium electronic structure with tunable energy and time resolution [1], opening new pathways to investigate elementary and composite excitations in low-dimensional systems.
Using this approach, I will present recent results on van der Waals antiferromagnets, focusing on the interplay between orbital degrees of freedom, magnetic order, and ultrafast dynamics. First, I will discuss the electronic structure of the layered semiconductor $CrPS_4$, where ARPES combined with DFT reveals a ligand-to-metal charge-transfer gap and distinct hybridization regimes within the Cr 3d manifold, linking weakly hybridized t_2g states to magnetic order and strongly hybridized eg states to optically active orbital excitations [2].
Building on this microscopic framework, I will then show how time-resolved ARPES provides access to orbital d–d excitations in $FePS_3$ through their momentum-dependent photoemission signatures [3]. Although these excitations are intrinsically local and not dispersive in a band-structure sense, their spectral fingerprints exhibit a well-defined structure in momentum space. By resolving their dynamics, we identify fundamentally different relaxation pathways for spin-allowed and spin-forbidden transitions, governed by exchange interactions and spin–orbit coupling.
Together, these results establish momentum-resolved photoemission as a versatile approach to uncover the signatures of ultrafast orbital excitations and their coupling to other degrees of freedom [4], paving the way toward a microscopic understanding of composite excitations in correlated quantum materials.

[1] K. Schiller, et al. Scientific Reports 15:3611 (2025). doi:10.1038/s41598-025-86660-1
[2] L. Sternemann, L., et al. arXiv (2025). doi:10.48550/arxiv.2511.17403
[3] J. E. Nitschke, et al. Newton 1, 100019 (2025). doi:10.1016/j.newton.2025.100019
[4] F. Mertens, Advanced Materials 35, 2208355 (2023). DOI:10.1002/adma.202208355

642	**Ultrafast exciton dynamics in metal-phthalocyanine/WSe_2 heterostructures**	Gregor Zinke	Contributed talk (17:45-18:00)

Gregor Zinke (1) Martin Anstett (2) Sebastian Hedwig (2) Benito Arnoldi (2) Martin Aeschlimann (2) Benjamin Stadtmüller (1)

(1) University of Augsburg
(2) RPTU Kaiserslautern-Landau

Two-dimensional (2D) van der Waals materials and their heterostructures with molecular materials are a highly promising class of materials due to their low dimensional nature and highly tuneable electronic properties that lead to rich charge and spin carrier dynamics. Beyond chemical tunability, their optoelectronic properties can be dynamically modified on ultrafast timescales through the formation of transient charge-separated states. [1]
In this work, we investigate hybrid heterostructures consisting of metal phthalocyanine (MPc) molecular films deposited on bulk transition metal dichalcogenides (TMDCs), specifically a FePc monolayer on WSe_2. Interfacial interaction leads to an altered energy level alignment in the electronic band structure, with the FePc HOMO sitting in between the spin-split valence states of WSe. Additionally, the distinct orbital character of the iron centre induces a long-range ordering of the molecular layer, resulting in a localisation of molecular bands in momentum space.
Building on this, we explore the optically induced ultrafast charge carrier dynamics using time- and angle-resolved photoemission spectroscopy (trARPES) in a VIS-pump, XUV-probe scheme. This approach enables us to simultaneously track excited electron populations and the corresponding hole dynamics on femtosecond timescales. By disentangling intra- and interlayer processes via their distinct momentum-space signatures, we reveal the temporal evolution of

charge transfer across the FePc/WSe_2 interface, demonstrating how transient charge separation leads to ultrafast modifications of the interfacial energy-level alignment.

[1] B. Arnoldi et al., Nat.Commun. 15, 3573 (2024)

M20 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
579 **P021**	**Electronic Band Engineering in Two-Dimensional Bimetallic Metal-Organic Frameworks**	Maedeh Hakimi	Poster

Y. Y. Grisan Qiu (1) Maedeh Hakimi (2) D. Brandstetter (2) C. Di Giorgio (3) T. Zio (3) S. Mearini (1) P. Puschnig (2) V. Feyer (1) C. M. Schneider (4)

(1) Peter Grünberg Institute (PGI-6), Jülich Research Centre, 52428 Jülich, Germany
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(3) CNR-IOM, Lab. TASC, s.s. 14 km 163,5, 34149 Trieste, Italy
(4) Faculty of Physics and Center for Nanointegration Duisburg-Essen (CENIDE), University of Duisburg-Essen, 47048 Duisburg, Germany

Two-dimensional metal-organic frameworks offer a highly versatile platform for designing novel electronic materials. Their electronic band structures are typically constrained by rigid framework compositions dictated by the discrete identities of the constituent metal ions and organic ligands[1]. Achieving continuous electronic tunability requires the development of structurally invariant but compositionally variable coordination lattices[2]. Utilizing a tetracyanoquinodimethane (TCNQ)-based network grown on a Ag(100) surface, a mixed-metal bimetallic framework can be achieved through sequential metal incorporation. An initial, partially coordinated Ni-TCNQ structure is saturated with a second transition metal species, specifically Cobalt, forming a fully coordinated two-dimensional network resulting in a two-dimensional Ni-Co coordinating alloy.
Scanning tunnelling microscopy and low-energy electron diffraction verify that the low-valence Ni and Co transition metal centers occupy equivalent molecular coordination sites while preserving the long-range crystalline order of the parent lattice. Momentum-resolved photoemission spectroscopy demonstrate a significant influence of the bimetallic mixing on the dispersive electronic band structure of the hybridisation network. The macroscopic bandwidth and the band curvature evolve systematically as a direct function of the transition metal composition ratio. This compositional flexibility enables the quantitative control of the charge carrier effective mass and intrinsic dispersive properties without disrupting the inherent electronic delocalization of the two-dimensional molecular network.

[1] D. Baranowski et al. ACS Nano 18, 30 (2024)
[2] S. Mearini et al., Adv. Science 11, 38 (2024)

ID	Title	Presenter	Type
569 **P022**	**Single Ni Atoms Drive Carboxyl Deprotonation in Metal-Organic Chains**	Dominik Brandstetter	Poster

Dominik Brandstetter (1) Fabian Auer (1) Daniel Baranowski (2) Iulia Cojocariu (3,4) Vitaliy Feyer (2,5) Yan Yan Grisan Qiu (2) Matteo Jugovac (3,4) Maximilian Laßhofer (1) Simone Mearini (2) Claus Michael Schneider (2,5,6) Martin Sterrer (1) Andreas Windischbacher (1) Giovanni Zamborlini (1)

(1) Institute of Physics, University of Graz, 8010 Graz, Austria
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(6) Department of Physics and Astronomy, UC Davis, Davis CA 95616, USA

On-surface synthesis of low-dimensional metal-organic architectures provides a versatile platform to create ordered assemblies with tuneable structural and electronic properties [1,2]. One vector for this flexibility lies in the choice of the active functional groups bonding with the metal atoms. Among them, carboxyl (-COOH) groups are particularly interesting because they can coordinate in both a mono- and bi-dentate manner as well as host a strong nucleophilic site. Uphoff et al. have shown a possible route for activating these carboxylate groups through deprotonation, by employing a hot-deposition step in the formation of a TPA-based MOF using Ho atoms on Ag(100) [3]. It remains unclear whether this requirement of pre-activation is intrinsic to TPA or if the incorporation of a different metal atom can directly promote ligand deprotonation without prior substrate-induced activation. We address this question using scanning tunnelling microscopy, X-ray photoelectron and valence band spectroscopy, complemented by density functional theory calculations.
We investigate metal-organic coordination by examining nickel atoms interacting with a preassembled hydrogen-bonded terephthalic acid (TPA) monolayer on Ag(100), for which we explicitly do not follow the hot-deposition step outlined by Uphoff et al. [3] and find the majority of ligands still in the protonated carboxyl state. Upon Ni incorporation, X-ray photoelectron spectroscopy unambiguously reveals Ni(I) centers stabilized by a single-electron charge transfer process, as well as a quenching of the -COOH peak, clearly demonstrating the direct deprotonation of the previously inactive TPA ligands. The resulting formation of an extended metal-organic framework is further confirmed by valence band spectroscopy showing coordination-induced electronic reorganization between Ni and TPA via emergent hybrid states [4]. Furthermore, we find that the +1 oxidation state of Ni, together with the network structure, fundamentally limits the Ni-induced deprotonation to 50%. Our results demonstrate that charge-transfer-driven deprotonation is the central mechanism for linear metal-organic chain formation, deepening the understanding of structural motifs and electronic properties in low-dimensional systems.

[1] S. Mearini et al., Adv. Science 11, 38 (2024)
[2] S. Mearini et al., Small 21, 12 (2025)
[3] M. Uphoff et al., ACS Nano 12, 11 (2018)
[4] D. Baranowski et al. ACS Nano 18, 30 (2024)

M21 - Recent Developments in Machine Learned Interatomic Potentials

M21 – Session 1 (Wed 23, 10:30-12:30, Chair: Egbert Zojer)			
ID	Title	Speaker	Type
739	**From Specialized to Foundational: Machine Learning Interatomic Potentials at Scale**	Ralf Drautz	Invited talk (10:30-11:00)

Ralf Drautz (1)

(1) ICAMS/Ruhr-Universität Bochum

Machine Learning Interatomic Potentials (MLIPs) are undergoing a paradigm shift from narrowly trained, system-specific models to universal frameworks intended to generalize across the periodic table. While early MLIPs focused on accelerating atomistic simulations for a particular material or chemistry, recent developments emphasize capturing complex thermodynamic and kinetic properties in arbitrary material compositions.
This presentation introduces the Graph Atomic Cluster Expansion (GRACE) and explains how its underlying architecture enables accurate, large-scale simulations of complex material compositions. By efficiently managing the combinatorial explosion inherent to multi-component systems, GRACE preserves linear scaling with system size. The completeness of the underlying basis expansion makes GRACE not only a model but a unifying framework: a wide range of existing MLIP architectures can be recovered as special cases, and the same completeness enables principled extensions to interactions involving dynamic charge transfer and magnetism that have historically challenged conventional atomistic models.
Model accuracy is ultimately bounded by training data, and conventional datasets carry strong thermodynamic and chemical bias toward near-equilibrium structures. GRACE counters this with uncertainty-driven, maximum-entropy, chemistry-agnostic sampling, decoupling structural generation from thermodynamic constraints and establishing a broad physical prior. We demonstrate this on stable molecular dynamics simulations at high temperature and pressure containing more than 90 chemical species simultaneously in a single simulation, resolving emergent structures in complex mixtures — such as high-entropy alloys — without a priori chemical assumptions.

604	**Exploring Data-Efficient Fine-Tuning and Training Strategies for Accurate Machine-Learning Interatomic Potentials**	Jonas Hänseroth	Contributed talk (11:00-11:15)

Jonas Hänseroth (1) Christian Dreßler (1)

(1) Technische Universität Ilmenau

This work demonstrates that systematic fine-tuning transforms modern foundation machine-learned interatomic potentials (MLIPs) into consistently accurate, near-ab initio models across diverse architectures. Benchmarking five leading frameworks-MACE, GRACE, SevenNet, MatterSim, and ORB-we show that fine-tuning improves force and energy predictions by up to one and three orders of magnitude, respectively, while largely eliminating architecture-dependent performance differences.
Beyond benchmarking, we systematically explore the roles of training strategy and data composition by comparing fine-tuning with training-from-scratch across varying dataset sizes. In particular, we investigate the impact of data generated via short ab initio molecular dynamics trajectories alongside structures obtained from foundation-model-driven simulations and subsequently recalculated with density functional theory. This unified perspective reveals how dataset origin and size jointly control accuracy, efficiency, and transferability.
Focusing on rare-event systems involving bond breaking, formation, and high energy barrier transitions, we develop simple, robust, and systematically improvable protocols that remain effective even in data-limited regimes. We further demonstrate an iterative fine-tuning approach, where model-driven sampling and retraining progressively refine accuracy, enabling efficient exploration of challenging regions of configuration space.
These strategies yield harmonized performance across architectures while maintaining computational efficiency and enabling realistic simulations of degradation reactions in fuel cells under operating conditions. To facilitate adoption, we introduce the aMACEing Toolkit, providing unified and reproducible workflows for both fine-tuning and training-from-scratch.

770	**Complex Configurations with Quantum Accuracy: Dynamics of Molecular Liquids from a General-Purpose Machine-Learned Potential**	Florian Brünig	Contributed talk (11:15-11:30)

Florian Brünig (1) Adil Kabylda (1) Alexandre Tkatchenko (1)

(1) University of Luxembourg

Liquids provide a uniquely stringent test for atomistic modeling: experimentally accessible observables such as structure factors, diffusion coefficients, and vibrational spectra emerge from a delicate interplay of quantum-mechanical intermolecular interactions, collective fluctuations, and nuclear quantum effects over extended length and time scales. Still, these properties remain challenging to predict from first principles because accurate liquid simulations require both quantum-level interaction models and extensive statistical sampling. While conventional force fields are often parametrized directly against experimental data, limiting their value as predictive models, transferable machine-learning force fields offer the possibility of genuinely bottom-up simulations with experiment serving as an independent benchmark.
Here, we present recent developments of SO3LR [1], a machine-learned interatomic potential that combines the efficient SO3krates architecture [2] for short-range interactions with physically motivated long-range electrostatics and dispersion, pretrained on a broad dataset of molecular complexes. With JAX acceleration, SO3LR makes nanosecond-scale simulations of thousands of atoms feasible at low cost. Leveraging this efficiency and stability, we perform extensive molecular and path-integral dynamics of representative liquids, yielding converged structural, dynamical, and vibrational observables with realistic conformational sampling and full anharmonicity.
Direct comparison with experimental vibrational spectra and other liquid-phase data allows us to evaluate the predictive accuracy of the underlying quantum description and disentangle intrinsic limitations of classical force fields. Our results demonstrate that transferable machine-learning force fields can bridge the gap between empirical models and ab initio methods, enabling predictive simulations of condensed-phase systems with quantum-mechanical accuracy at experimentally relevant scales.

[1] Kabylda, A. et al. JACS 147, 33723–33734 (2025).
[2] Frank, J.T. et al. Nat Commun 15, 6539 (2024).

737	**Self-Consistent Fine-Tuning of Machine Learning Interatomic Potentials by Targeted Exploration of Configuration Space**	Julien Steffen	Contributed talk (11:30-11:45)

Julien Steffen (1)

(1) Lehrstuhl für Theoretische Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg

Universal machine learning interatomic potentials (uMLIPs) have shown an astonishing ability of describing almost arbitrary chemical systems reasonably. They are, however, not accurate enough for the calculation of quantities like reaction rate constants that require a very precise representation of the potential energy surface. Fortunately, uMLIPs can be fine-tuned for a system of interest, by training them on system-specific ab initio reference data. The generation of such reference data is nontrivial since it requires a broad sampling of the relevant configuration space, often out of each for direct ab initio molecular dynamics (AIMD) [1]. Self-consistent fine-tuning is a solution for this: long MD samplings are done with the uMLIP, a relevant subset of sampled structures is recalculated with the ab initio method, and this is iterated with the successively fine-tuned MLIP to cure the slightly incorrect configurational sampling of the uMLIP [2].
In this contribution, I show how self-consistent fine-tuning of uMLIPs can be combined with umbrella samplings along complex reaction coordinates with the Caracal program package [3]. This enables the black-box setup of highly accurate targeted MLIPs for different chemical reaction mechanisms in arbitrary environments. I present the application of this method on a benchmark study of small proton exchange reactions in the gas phase [4], and then continue with real-world applications - based on actual ab initio data - for larger gas phase systems and hydrogen diffusions on different metal surfaces. In all examples, ring polymer molecular dynamics (RPMD) is used to consider nuclear quantum effects. Finally, an outlook is given on how to generalize the method to arbitrary chemical systems and reaction mechanisms.

[1] J. Steffen, A. Alibakhshi, J. Chem. Phys. 161, 184116 (2024).
[2] J. Steffen, J. Phys. Chem. C, 129, 13513 (2025).
[3] J. Steffen, J. Chem. Theory Comput., 19, 5334 (2023).
[4] J. Steffen, submitted (DOI: 10.26434/chemrxiv.15002012/v1).

364	**Mechanical and thermal properties of complex materials from machine-learned interatomic potentials**	Florian Lindner	Contributed talk (11:45-12:00)

Florian Lindner (1) Caterina Czibula (2) Lukas Legenstein (3) Marco Moser (1) Sandro Wieser (4) Egbert Zojer (1)

(1) Institute of Solid State Physics, Graz University of Technology
(2) Department of Materials Science and Engineering, Northwestern University
(3) Technical University of Leoben
(4) Institute of Materials Chemistry, TU Wien

Metal-organic frameworks (MOFs) are highly porous, mostly crystalline materials that hold considerable promise for addressing major societal challenges, for example in gas storage (CO_2 capture) and separation.[1] For many of these applications, mechanical response and thermal transport are key material properties.[2] As MOFs are typically insulating materials, both properties are governed by lattice vibrations. However, their quantitative prediction is challenging, as their structural complexity and large unit cells place them beyond the reach of routine density functional theory (DFT) simulations. This is particularly severe for observables such as thermal conductivity that require long molecular dynamics simulations of large supercells in order to account for finite size effects.
In recent years, machine-learned interatomic potentials (MLIPs) have emerged as powerful tools combining near-DFT accuracy with the efficiency needed to access the length and time scales relevant for simulating properties of complex materials.[3]
In this contribution, we show how MLIPs enable the investigation of both mechanical and thermal properties in complex materials like MOFs. For mechanical properties, we focus on long-wavelength limit properties i.e. elastic tensors.[4] We combine MLIP-based simulations with Brillouin light scattering (BLS),[5] a contactless, non-invasive spectroscopic technique that measures direction-dependent sound velocities and thereby provides access to the elastic tensor. This combined approach not only provides experimental validation of MLIP predictions for complex materials, but also demonstrates the potential of MLIPs as powerful tools for interpreting BLS measurements, particularly in structurally complex, disordered, or glassy systems.
We then extend this perspective to thermal transport in MOFs. While MLIPs enable detailed insights into heat-transport mechanisms through reciprocal-space analyses based on phonon transport formalisms,[6,7] we focus here on a complementary real-space approach: Green-Kubo (GK) theory.
This is particularly relevant also for cases in which a simple phonon picture might become less useful, for example in the case of freely moving guest molecules within the pores of a MOF. For such cases, GK simulations provide a powerful framework, but their application is often hindered by statistical noise and slow convergence. We show that this problematic can be overcome elegantly by applying Cepstral analysis to GK-based transport calculations, significantly improving both their efficiency and their reliability.[8] Quantitative comparison with single-crystal experiments for MOF-5 and HKUST-1 reveals excellent agreement with the predicted thermal conductivities.[9]
This is of considerable practical importance, because recent progress in MLIPs increasingly points toward more expressive and transferable architectures, often at the cost of computational speed. The substantially reduced simulation times enabled by cepstral-analysis-based GK simulations make the use of such more advanced MLIPs feasible also for more realistic scenarios involving for example guest molecules or defects. Taken together, these results demonstrate how MLIPs are evolving into powerful tools for the quantitative exploration of vibrationally governed properties in complex materials beyond the reach of direct DFT simulations.

[1] J.-B. Lin, T. T. T. Nguyen, R. Vaidhyanathan, J. Burner, J. M. Taylor, H. Durekova, F. Akhtar, R. K. Mah, O. Ghaffari-Nik, S. Marx, N. Fylstra, S. S. Iremonger, K. W. Dawson, P. Sarkar, P. Hovington, A. Rajendran, T. K. Woo, G. K. H. Shimizu, Science 2021, 374, 1464.
[2] N. C. Burtch, J. Heinen, T. D. Bennett, D. Dubbeldam, M. D. Allendorf, Adv. Mater. 2018, 30, 1704124.
[3] S. Wieser, E. Zojer, Npj Comput. Mater. 2024, 10, 18.
[4] F. P. Lindner, N. Strasser, M. Schultze, S. Wieser, C. Slugovc, K. Elsayad, K. J. Koski, E. Zojer, C. Czibula, J. Phys. Chem. Lett. 2025, 16, 1213.
[5] I. Kabakova, J. Zhang, Y. Xiang, S. Caponi, A. Bilenca, J. Guck, G. Scarcelli, Nat. Rev. Methods Primer 2024, 4, 8.
[6] Florian P. Lindner, Marco Moser, Lukas Legenstein, Sandro Wieser, Egbert Zojer, in preparation;
[7] L. Legenstein, L. Reicht, S. Wieser, M. Simoncelli, E. Zojer, Npj Comput. Mater. 2025, 11, 29.
[8] S. Wieser, Y.-J. Cen, G. K. H. Madsen, J. Carrete, J. Chem. Theory Comput. 2026, 22, 513.
[9] Florian P. Lindner, Egbert Zojer, and Sandro Wieser, in preparation;

388	**Learning Long-Range Electrostatics via Born Effective Charges in Atomistic Machine Learning**	Angela Rittsteuer	Contributed talk (12:00-12:15)

Angela Rittsteuer (1) Anton Bochkarev (2) Ralf Drautz (2) Tobias Hilpert (1) Georg Kresse (1) Bernhard Schmiedmayer (1)

(1) University of Vienna
(2) Ruhr University Bochum

Most atomistic machine-learning models rely on local atomic representations with finite spatial cutoffs and therefore struggle to capture long-range electrostatic effects. To address this limitation, we build on the fact that Born effective charges, defined as derivatives of the macroscopic polarization with respect to atomic displacements, provide a well defined description of the coupling between atomic structure and long-range electrostatic response. Unlike the macroscopic polarization itself, which is only defined modulo a polarization quantum in periodic systems, Born effective charges are unambiguous response quantities.
In our approach, local polarization dipoles are learned and constrained such that their derivatives reproduce the Born effective charges, and embedded in an explicit long-range electrostatic energy expression learned alongside the short-range part of the model, providing a consistent framework for coupling local atomic structure to long-range electrostatic interactions.We implement this within the Graph Atomic Cluster Expansion (GRACE), and demonstrate that the resulting model reduces prediction errors and mitigates finite-size effects, enabling models trained on small simulation cells to generalize to larger systems. Results are shown for representative material systems.

M21 – Session 2 (Wed 23, 16:00-18:00, Chair: Christian Dreßler)

ID	Title	Speaker	Type
766	**Transition-Point Sampling via Stochastic Saddle Point Dynamics for Training Machine-Learned Interatomic Potentials**	Sandro Wieser	Invited talk (16:00-16:30)

Sandro Wieser (1)

(1) Institute of Materials Chemistry, TU Wien

Dataset generation is a critical component for obtaining accurate machine-learned interatomic potentials (MLIPs). Molecular dynamics is widely used for reference data generation; however, it struggles to sample rare events such as transition states. This limitation is particularly problematic when fine-tuning foundation models, in which such configurations are typically underrepresented.
To address this challenge, we employ a recently developed algorithm, stochastic saddle point dynamics (SSPD) [1,2] to generate reference configurations without relying on predefined collective variables. This approach steers Langevin dynamics toward transition states, enabling efficient sampling not only at but also in the vicinity of these configurations. The use of SSPD has recently been demonstrated for identifying transition states in the decomposition of isopropanol and CO dissociation on Co surfaces [3].
Here, we apply SSPD to generate reference data near transition states associated with oxygen ion migration in perovskites. We demonstrate its capability to sample configurations close to transition states in $SrTiO_{3-\delta}$, enabling efficient fine-tuning of MACE foundation models to accurately predict migration barriers at the target level of theory. Furthermore, SSPD-driven active learning is used to perform larger-scale investigations of the more complex $La_{1-x}Sr_xFeO_{3-\delta}$ system across varying Sr concentrations. We observe substantial variations in migration barriers depending on the migration pathway, revealing a more intricate landscape than previously assumed for identifying efficient transport routes. Overall, SSPD provides a powerful addition to the dataset generation toolkit, addressing a key limitation of conventional approaches.

[1] S. Tănase-Nicola et al., 10.1103/PhysRevLett.91.188302
[2] T. Lelièvre et al., 10.1137/22M1541964
[3] M. Ketter et al., 10.26434/chemrxiv-2025-1psv7

ID	Title	Speaker	Type
73	**High-Throughput ML-accelerated Exploration of Conformal Funnels in NanoCatalysis**	Alessandro Fortunelli	Contributed talk (16:30-16:45)

Alessandro Fortunelli (1) Thantip Roongcharoen (1)

(1) Italian National Research Council (CNR)

I will present our methodological advances in the computational modeling of dynamical processes in chemistry and materials science, and how they are enabling us to address the dramatically urgent societal pressure toward a 'green chemistry' that can help solve global energy and environmental issues and establish environmentally sustainable matter/energy cycles.
Our strategy combines stochastic sampling methods, such as Global Optimization and Reactive Global Optimization, exploring both structural and compositional degrees of freedom, with Potential Energy Surface (PES) interpolation via Machine Learning acceleration grounded on physical principles [1-3]. I will show how this two-fold approach is indispensable due to the arithmetically rugged landscape of the chemical space, ultimately a result of the intrinsic quantum structure of matter, that requires a synergy of rational design and high-throughput screening pushed to the extreme. Accelerating first-principles-level modeling to enable high-throughput processing of millions of material candidates is then made possible by empowering the stochastic search with both Artificial Intelligence techniques and rational design strategies exploiting physical domain knowledge, such as conformal/homothetic and reaction-energy-invariant transformations, and transfer of accumulated knowledge. This leads to the predictive investigation of long time- and length-scale phenomena, in advance but crossvalidated and strictly interacting with experiment.

[1] T. Roongcharoen, G. Conter, L. Sementa, G. Melani, A. Fortunelli "Machine-Learning-Accelerated DFT Conformal Sampling of Catalytic Processes" J. Chem. Theory Comput., 2024, 20(21), 9580-9591, DOI: 10.1021/acs.jctc.4c00643; cover: https://pubs.acs.org/toc/jctcce/20/21.
[2] T. Roongcharoen, G. Conter, L. Sementa, G. Melani, A. Fortunelli "Machine-Learning-Accelerated Conformal Sampling of Methanol Catalytic Conversion on Bimetallic Systems" J. Chem. Phys. C, 2025, 129(39), 17472-17483; DOI: 10.1021/acs.jpcc.5c00825.
[3] T. Roongcharoen, G. Conter, G. Melani, L. Sementa, A. Fortunelli "Extrapolation Techniques in Database Construction for Machine-Learning Potentials Achieving Sub-Chemical Accuracy in Sampling Conformal Funnels in Catalytic Processes" J. Chem. Theory Comput., 2025, 21(21), 11164-11178, DOI: 10.1021/acs.jctc.5c00860; cover: https://pubs.acs.org/toc/jctcce/21/21.

ID	Title	Speaker	Type
610	**Machine Learning Interatomic Potentials for Cooperative Sulfur Vacancy Dynamics in Two-Dimensional MoS_2**	Aaron Flötotto	Contributed talk (16:45-17:00)

Aaron Flötotto (1) Erich Runge (1) Christian Dreßler (1)

Technische Universität Ilmenau

The memristive properties of transition metal dichalcogenides, such as MoS_2, have attracted significant attention and have recently been linked to the dynamics of sulfur vacancies [1, 2]. However, the inherently slow kinetics of sulfur vacancy migration in MoS_2 renders direct ab initio simulations computationally infeasible. To overcome this limitation, we train both graph neural network machine-learning interatomic potentials (MLIPs) and Gaussian approximation potentials for this system. Beyond systematically evaluating model architectures and training strategies, we emphasize the importance of validating physically relevant observables—specifically diffusion barrier heights—rather than relying solely on conventional metrics such as energy and force errors on randomly sampled test sets prior to molecular dynamics (MD) simulations. Nanosecond-scale MD simulations applying the resulting MLIP reveal key mechanisms of cooperative vacancy transport providing a coherent explanation of irradiation-induced vacancy patterns, especially the formation of line defects spanning tens of nanometers [3].

[1] D.Li, B.Wu, X.Zhu, J.Wang, B.Ryu, W.D.Lu, W.Lu, X.Liang, "MoS_2 Memristors Exhibiting Variable Switching Characteristics toward Biorealistic Synaptic Emulation", ACS Nano 12 (2018): pp. 9240–9252. https://doi.org/10.1021/acsnano.8b03977.
[2] B.Spetzler, D.Abdel, F.Schwierz, M.Ziegler, P.Farrell, "The Role of Vacancy Dynamics in Two-Dimensional Memristive Devices", Adv. Electron. Mater. 10 (2023): 2300635. https://doi.org/10.1002/aelm.202300635
[3] A.Flötotto, B.Spetzler, R.von Stackelberg, M.Ziegler, E.Runge, C.Dreßler, "Large-Scale Cooperative Sulfur Vacancy Dynamics in Two-Dimensional MoS_2 From Machine Learning Interatomic Potentials", Small 20 (2026): e10679. https://doi.org/10.1002/smll.202510679

638	**Versatile correlated frozen phonons from universal MLIPs for (S)TEM/EELS simulations**	Toma Susi	Contributed talk (17:00-17:15)

Toma Susi (1) Adam Jackson (2) Jan Rusz (3) Naoya Shibata (4) Koudai Tabata (4) Paul Zeiger (5)

(1) University of Vienna
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Harmonic phonon modes are not only critical for understanding the thermal properties of materials, but also desirable for accurate transmission electron microscopy simulations within the widely-used frozen-phonon approach. Although uncorrelated random displacements are typically sufficient for modeling diffuse backgrounds [1], the true correlated phonons may be of relevance for techniques including quantitative electron diffraction and electron ptychography [2] – and vital for simulating momentum-resolved ultra-low electron energy-loss spectroscopy (EELS).
Although ab initio methods are routinely applied to calculate phonon dispersions for small and often non-orthogonal unit cells, (scanning) transmission electron microscopy ((S)TEM) scattering simulations typically require atomic displacements for potentially quite large orthogonal supercells. Further, since both the technical and computational effort of accurately simulating phonons from first principles is often greater than that of scattering, this severely limits their accessibility and adoption by the electron microscopy community.
This challenge can be overcome with the help of force-constant potentials [3], which allow phonon properties learned for small cells to be extrapolated to arbitrary supercells. In this way, correlated phonon displacements for a given specimen model can be easily generated – including quantum-mechanical zero-point motion that is increasingly important as cryogenic instrumentation becomes more widespread. To further enhance the universality of this approach, the required forces can be efficiently calculated using recently developed foundational machine-learning interatomic potential (MLIPs), which have very recently become sufficiently accurate to model harmonic phonons for many materials across the periodic table [4].
In this contribution, we establish a fully Python-based high-performance open-source workflow for including ab initio frozen phonons in electron scattering simulations using the abTEM package [5]. As demonstrations of our versatile approach, we quantify the effect of phonon correlations for selected-area and convergent-beam electron diffraction of SrTiO, and reproduce experimentally measured momentum-resolved phonon-loss EEL spectra for graphene and hBN, using a new mode-selective rattle to efficiently generate the required frequency-resolved snapshots [6].
Finally, we apply our methodology to accurately model phonon-dependent electron scattering in silicon to show how correlated thermal motion between neighboring atoms preserves coherence even at elevated temperatures. Experimentally, this enables atomic-scale double-slit interferometry with a focused electron probe transmitting through a thin silicon crystal [7].

393	**Using machine-learned interatomic potentials for accurate thermal conductivity predictions via non-equilibrium molecular dynamics**	Florian Unterkofler	Contributed talk (17:15-17:30)

Florian Unterkofler (1) Lukas Legenstein (2) Sandro Wieser (3) Egbert Zojer (1)

(1) Institute of Solid State Physics, Graz University of Technology
(2) Montanuniversität Leoben
(3) Institute of Materials Chemistry, TU Wien

With the rise of machine-learned interatomic potentials, simulations have become an even more crucial tool for predicting material properties. We previously achieved accurate predictions of experimentally observed thermal conductivity of acenes, using system-specific, machine-learned Moment Tensor Potentials (MTPs) within a lattice dynamics approach.[1] To obtain a complementary real-space perspective, we now investigate whether comparable accuracy can be achieved using non-equilibrium molecular dynamics (NEMD).
Here, we present the workflow required to obtain accurate and reliable predictions when applying MTPs in NEMD simulations. We show that, due to the inherently stochastic nature of both MD and MTP training, a thorough statistical analysis of multiple simulations with different initial conditions and different realizations of the MTP is necessary. Furthermore, we highlight the importance of selecting appropriate training data to generate robust MTPs.
When these considerations are taken into account, we achieve an excellent agreement between experiments, lattice-dynamics, and NEMD results, with NEMD simulations providing tools to investigate heat-transport bottlenecks in real space.

[1] L. Legenstein et al., npj Comput Mater 11, 29 (2025)

717	**Unraveling Polymorphism and Heat Transport in Hydrogen-Bonded Molecular Crystals using MACE Models**	Lukas Legenstein	Contributed talk (17:30-17:45)

Lukas Legenstein (1) Sandro Wieser (2) Michele Simoncelli (3) Egbert Zojer (4)

(1) Montanuniversität Leoben
(2) Institute of Materials Chemistry, TU Wien
(3) Columbia University, NY
(4) Institute of Solid State Physics, Graz University of Technology

Polymorphism, the ability of molecules to form solid phases with slightly different arrangements, profoundly influences the material properties of molecular crystals in both pharmaceutics and organic electronics. Even minor variations in molecular packing can lead to vastly different charge transport properties in organic semiconductors. Indicative of this phenomenon are also subtle differences in the relative energies of polymorphic phases, often on the order of just a few meV. Accurately capturing these fine energy distinctions is challenging, as the uncertainty in machine-learned potentials (MLPs) can exceed the energy differences between polymorphs. We focus on systems such as quinacridone, a pentacene derivative, where the hetero-atom substitution facilitates categorically different hydrogen bonding motifs. Despite their unique structures, the energy variations between two of these polymorphs are as small as 0.1 meV/atom.
To model such systems, we are developing a workflow to train MLPs that can accurately capture these subtle energy differences to describe diverse polymorphic phases. Specifically, we are testing three training strategies for general MACE models: (1) naïve training on mixed datasets of three primary polymorphs, (2) training a multi-head model with cross-learning between polymorph-specific heads, and (3) finetuning foundation models to specialize in these systems.
The most effective model from this investigation is then applied to predict the thermal conductivities of three individual polymorphs using the Wigner transport framework. By comparing these predictions on equal footing, we aim to uncover how polymorphism and the accompanying structural variations impact heat transport in hydrogen-bonded molecular crystals. Additionally, this work provides valuable strategies for designing highly accurate MLPs for advanced modeling applications in organic electronics and pharmaceuticals.

479	**Machine-Learning Supported Reaction Mechanism Exploration of cis-trans Isomerisation in Retinal**	Kai Töpfer	Contributed talk (17:45-18:00)

Kai Töpfer (1) Bettina G. Keller (1)

(1) Freie Universität Berlin

Rare events such as chemical reaction are transitions across an energy barrier. To rationalize the mechanism of such rare events and calculating their reaction rates, the search for an optimal reaction coordinates has long been very active field of research.[1] Using the minimum energy path (MEP) as reaction coordinate simply neglects entropic contributions and dynamic effects. Alternatively, the committor function offers a complementary perspective in which the transition state is defined as an isocommittor surface at which trajectories reach the reactant or product with equal probability.
I will present our findings on the reaction mechanism of the cis-trans isomerization of retinal in gas phase and various solvation environments.[2] We apply the recently developed AIMMD algorithm,[3] where the committor of isomerization reaction is learned by a Neural Network (NN) function from short, dynamically unbiased trajectories that form a transition path ensemble (TPE) and are generated by two-way shooting molecular dynamics (MD) simulations. MD simulations are performed using self-developed machine-learned interaction potentials (MLIPs) and adaptively trained universal MLIPs to provide ab initio accuracy for comparatively low computational costs.[4] The low-dimensional approximation of committor function is obtained through symbolic regression, which yields a human-interpretable reaction mechanism in terms of a small set of internal degrees of freedom.
We observe a significant deviation of the TPE from underdamped Langevin dynamics with time scales in the range of hundreds of femtoseconds compared to the MEP obtained from overdamped simulations in the nanoseconds regime. Overdamped simulations do not show the asymmetric distribution of kinetic energy along different internal coordinates at various stages of the isomerization reaction, as seen in the TPE. Such differences must be taken into account when calculating accurate reaction rates with respect to experimental results, e.g., transition state theory.[5]

[1] Chen, H.; Roux, B.; Chipot, C., J. Chem. Theory Comput. 2023, 19, 4414–4426
[2] Ghysbrecht, S.; Donati, L.; Keller, B. G., J. Comput. Chem. 2025, 46, e27529
[3] Jung, H.; Covino, R.; Arjun, A.; Leitold, C.; Dellago, C.; Bolhuis, P. G.; Hummer, G., Nat. Comput. Sci. 2023, 3, 334–345
[4] Käser, S.; Vazquez-Salazar, L. I.; Meuwly, M.; Töpfer, K., Digit. Discovery 2023, 2, 28–58
[5] Ghysbrecht, S.; Keller, B. G., J. Comput. Chem. 2024, 45, 1390–1403

M21 – Session 3 (Thu 24, 10:30-12:30, Chair: Christian Dreßler)

ID	Title	Speaker	Type
794	**Prokyon – A Free On-the-Fly Machine Learning Library based on Sparse Gaussian Processes**	Martin Brehm	Contributed talk (10:30-10:45)

Omid Shayestehpour (1) Hossam Elgabarty (1) Robert Schade (1) Christian Plessl (1) Christian Dreßler (2) Martin Brehm (1)

(1) Paderborn University, Warburger Straße 100, 33098 Paderborn, Germany
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We present Prokyon [1], a free software library that enables on-the-fly machine learning (ML) of interatomic potentials for atomistic simulations that can be efficiently coupled to existing electronic structure packages. Apart from the energy and forces, our model also predicts the uncertainty in these quantities, which is a major advantage of the Gaussian process (GP) approach used here when compared to, e. g., neural network models. By doing so, we can judge if a certain simulation step can be reliably predicted via ML. The ML model is initialized from scratch and trained iteratively on-the-fly in parallel with an ab initio molecular dynamics (AIMD) run, so that more and more steps can be reliably predicted as the simulation proceeds, leading to an increasing speedup of the simulation. Prokyon is designed as a modular framework for incorporating different ML approaches. The library currently includes an optimized implementation of the FLARE [2] model based on atomic cluster expansion (ACE) [3] descriptors and sparse Gaussian process regression (GPR). Initial testing shows that we can reach an accuracy which is at least on par with other existing on-the-fly ML approaches such as the one implemented in VASP [4]. Prokyon can be integrated into existing AIMD program packages, so that all the methods available in these packages can then be coupled to our ML protocol, opening the door to time scales which were previously out of scope for AIMD simulations. As a first step, Prokyon will be integrated into the CP2k [5] and ORCA [6] packages.

[1] https://prokyon-lib.org/
[2] J. Vandermause, S. B. Torrisi, S. Batzner, Y. Xie, L. Sun, A. M. Kolpak, B. Kozinsky,

npj Comput. Mater. 2020, 6, 20.
[3] R. Drautz, Phys. Rev. B 2019, 99, 014104.
[4] R. Jinnouchi, F. Karsai, G. Kresse, Phys. Rev. B 2019, 100, 014105.
[5] https://www.cp2k.org/
[6] https://orcaforum.kofo.mpg.de/

785	**Elucidating the Complex Chemistry and Importance of Quantum Effects in High-Performing Electrolyte Solutions using SE(3)-Equivariant Transformer Network Potentials**	Mark E. Tuckerman	Invited talk (10:45-11:15)

Mark E. Tuckerman (1,2,3,4)

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(2) Courant Institute of Mathematical Sciences, New York University, New York, NY 10014 USA
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(4) Simons Center for Computational Physical Chemistry at New York University, New York, NY 10003 USA

Candidate systems for next-generation battery electrolyte materials, such as deep eutectic solvents and ionic liquids, often suffer from the limitation of an empirical inverse relation between viscosity and conductivity, known as Walden's rule, which suppresses rates of charge transport and limits their electrochemical performance characteristics. An alternative to these ionic systems involves a class of systems known as concentrated hydrogen-bonded electrolytes (CoHBEs), which are structured, electrochemically stable and less volatile. CoHBEs can also be designed such that charge transport kinetics and solvent dynamics are largely decoupled in such a way as to break the viscosity-conductivity tradeoff implied by Walden's rule. The basic strategy for achieving this breakthrough performance is to leverage the Grotthuss transport mechanism by choosing organic molecular solvent species, such as imidazole, capable of supporting proton hops through a dynamic, amphoteric hydrogen-bond network along with redox-active molecules capable of reversibly exchanging protons with the solvent species and undergoing proton-coupled electron transfer (PCET) reactions with each other. Accurate modeling of the charge transfer reactions and proton transport properties that give rise to high charge conductivities in these electrolytes proves computationally challenging because of the need to perform lengthy condensed phase simulations, treating both the electronic and nuclear degrees of freedom quantum mechanically. I will demonstrate that such a modeling task can be efficiently achieved with the use of DFT-trained SE(3)-equivariant transformer network potentials (MLP) to accelerate path integral molecular dynamics (PIMD) simulations. We highlight the practical utility of this approach by using it to benchmark how well PIMD simulations employing different DFT exchange-correlation functionals reproduce the composition-dependent densities, diffusion coefficients, and electrical conductivities of mixtures consisting of imidazole and either levulinic or acetic acid. Even with the speedup afforded by our MLPs, PIMD simulations remain quite expensive. In order to render PIMD more computationally tractable, we introduce and benchmark the accuracy of a ring polymer contraction approach that leverages a computationally efficient short-range MLP to accelerate our PIMD simulations by an additional factor of four.

M22 - Compressing Complexity: Machine Learning in Hard and Soft Condensed Matter Physics

M22 – Session 1 (Mon 21, 16:00-18:00, Chair: Carina Karner)			
ID	Title	Speaker	Type
622	**Learning to cross barriers: Machine learning for rare event simulations**	Christoph Dellago	Invited talk (16:00-16:30)

Christoph Dellago (1) Alessandro Coretti (1) Sebastian Falkner (2) Pablo Montero de Hijes (1)

(1) Faculty of Physics, University of Vienna
(2) University of Augsburg

Rare transitions between long-lived states underlie many important processes in condensed matter, from nucleation to protein folding, yet their simulation remains challenging due to the vast separation of timescales involved. In this talk, I will discuss how machine learning can enhance rare event simulations. A central theme is the committor function, the ideal reaction coordinate, which can be iteratively learned from transition path sampling data and used to guide the generation of new reactive trajectories. Symbolic regression then distills interpretable analytical expressions that reveal the relevant collective variables driving the transition. Identifying the few collective variables that matter is essentially a problem of physically informed dimensionality reduction. Applied to ice nucleation, this approach shows that nucleus size alone provides a non-Markovian description of the process, while structural descriptors such as crystalline order and tetrahedrality yield an improved reaction coordinate. I will also discuss how conditioned normalizing flows can generate independent shooting points for transition path sampling, removing correlations between sampled paths and enabling parallelization of the sampling process.

441	**Efficient Partition Function Estimation via Coordinate Design and Surrogate-Guided Sampling**	Johannes Krondorfer	Contributed talk (16:30-16:45)

Johannes Krondorfer (1) Markus Aichhorn (2) Christian Binder (1) Andreas Hauser (1)

(1) Institute of Experimental Physics, Graz University of Technology, Graz, Austria
(2) Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

Accurate evaluation of partition functions in molecular and solid-state systems remains computationally challenging due to high dimensionality and expensive energy evaluations. We present two complementary approaches to address this problem.
First, we introduce ZoRRO, a framework based on tailored coordinate transformations into translational, rotational, and vibrational (TRV) degrees of freedom. This representation isolates physically relevant modes, leading to improved energy landscapes and more efficient integration. Within this framework, thermodynamic properties, diffusion coefficients, and molecular uptake in external structures can be computed in a unified manner.
Second, we develop Slice Monte Carlo, a surrogate-guided integration scheme inspired by nested sampling. By leveraging lower-cost surrogate models, such as machine-learned potentials or force fields, to guide exploration, the method enables efficient evaluation of partition functions. The approach is athermal and robust to surrogate misspecification; even partial structural information is sufficient to guide the integration and improve performance, enabling the use of high-level models.
Together, these approaches provide a scalable route to efficient and reliable thermodynamic integration in complex systems.

580	**A synergistic approach to the parameter exploration of soft matter systems**	Emanuele Locatelli	Contributed talk (16:45-17:00)

Emanuele Locatelli (1)

(1) University of Padova

Diverse soft matter systems offer the possibility to tune the rheological response by tailoring microscopic interactions; however, brute-forcing the exploration may be either impractical or extremely costly. Here, we present an efficient approach for the exploration of the parameter space of soft matter systems based on the synergistic combination of coarse-grained modeling, Brownian dynamics simulations and machine learning. As a case study, we choose DNA-based associative fluids and we employ a minimal coarse-grained model, whose predictions are compared to experimentally available rheological curves. The model exhibits a viscoelastic response, characterized by a cross-over from viscous to elastic behavior. Coupling simulations with Gaussian Process Regression and active learning, we explore the design space with high predictive accuracy. Benchmarking against experimental DNA hydrogel data demonstrates that the model captures essential rheological behavior in the strongly associated regime and defines clear limits of applicability.

447	**Learning Dynamics of Autoencoders on Ising model data**	Max Weinmann	Contributed talk (17:00-17:15)

Max Weinmann (1) Miriam Klopotek (1)

(1) University of Stuttgart

Consistent, abstract descriptions of learning dynamics in neural networks are still uncommon, yet such descriptions appear across many scientific fields. Consequently, predicting how dynamics change with different ML model parameters can fail dramatically, and preventing these failures is challenging. Reliable control therefore demands a deep understanding of mechanisms and conditions that enable learning for specific kinds of datasets. We study autoencoder architectures that succeed when they compress data into representations that capture the data's underlying physical concepts and then learn an inverse mapping to reconstruct the original physical inputs. Certain physical concepts are acquired in a particular sequence, determined by the representational complexity and the architecture's theoretical capacity. We evaluate generalization against strict theoretical baselines and analyze the information geometry, stability, and physical interpretability of the latent space throughout training.

609	**Normalizing Flows for Atomistic Simulations of Condensed Matter Systems**	Alessandro Coretti	Contributed talk (17:15-17:30)

Alessandro Coretti (1) Livia Bartók-Pártay (2) Christoph Dellago (1) Sebastian Falkner (3) Phillip L. Geissler (4) Georg K. H. Madsen (5) Nico Unglert (5)

(1) University of Vienna
(2) University of Warwick
(3) University of Augsburg
(4) University of California, Berkeley
(5) TU Wien

Within the framework of deep learning, generative models are receiving increasing attention due to their ability to generate independent samples starting from a set of training examples. Their application to statistical mechanics is particularly promising, given the difficulty of generating decorrelated samples from complex physical distributions. This has led to a growing line of research in which generative models, and in particular normalizing flows, are integrated directly into atomistic simulation workflows, with encouraging results in condensed matter systems.
In this talk, I will present two approaches in which normalizing flows can be fruitfully applied to condensed matter physics. In the first case [1], we investigate equilibrium simulations of liquid systems by exploring physically informed choices of source distributions that more closely resemble the target distribution. This enables more efficient sampling of equilibrium configurations and facilitates exploration of thermodynamic variables, as well as transformations between different representations of the same physical system.
In the second case [2], we propose the use of conditional normalizing flows to enhance nested sampling in condensed matter systems. By replacing rejection-based Monte Carlo steps, which often constitute the primary computational bottleneck, this approach significantly improves sampling efficiency while preserving accuracy in the estimation of thermodynamic properties.

[1] AC, S. Falkner, P. L. Geissler, and C. Dellago, The Journal of Chemical Physics 162, 184102 (2025).
[2] AC, N. Unglert, S. Falkner, L.B. Pártay, G.K.H. Madsen, C. Dellago, manuscript in preparation (2026);

M22 – Session 2 (Tue 22, 16:00-18:00, Chair: Markus Wallerberger)

ID	Title	Speaker	Type
74	**Machine learning latent orders from the two-particle vertex**	Sabine Andergassen	Invited talk (16:00-16:30)

Sabine Andergassen (1) Sebastian Hepp (1) Daniel Zabielski (1) Daniel Springer (1)

(1) TU Wien

We explore the ability of machine learning models to extract information encoded in the two-particle vertex Γ that generalizes across different quantum phases. To steer the model away from relying on global phase-specific patterns we employ a sub-sampling strategy that encourages the model to learn general features tied to the phase specific competition between kinetic energy and Coulomb repulsion. We show that an autoencoder trained only on data from antiferromagnetic and ferromagnetic phases is able to reconstruct samples from a previously unseen superconducting phase. This demonstrates that the model captures essential aspects of the underlying many-body physics.

64	**Neural ODEs for Reduced-Order Quantum Many-Body Dynamics: Assessing Memory Effects**	Patrick Egenlauf	Contributed talk (16:30-16:45)

Iva Brezinova (1) Sabine Andergassen (1) Miriam Klopotek (2)

(1) TU Wien
(2) University of Stuttgart

Describing out-of-equilibrium quantum many-body dynamics remains a central challenge in condensed matter physics. While the time-dependent two-particle reduced density matrix (TD2RDM) formalism avoids the exponential scaling of exact wave-function methods, it requires closing the BBGKY hierarchy by reconstructing the three-particle cumulant. However, the validity of time-local reconstruction functionals - which ignore memory effects - remains unclear across different dynamical regimes.
In this work, we employ neural ordinary differential equations (ODEs) as a model-agnostic diagnostic tool to map the applicability of time-local cumulant expansion methods [1]. We show that neural ODEs trained on exact 2RDM data successfully extrapolate dynamics only when the correlation between two- and three-particle cumulants is high. In anti-correlated or uncorrelated regimes, the model's failure indicates that no time-local functional can capture the evolution, highlighting the necessity of memory-dependent kernels. These findings establish neural ODEs as a powerful diagnostic tool for mapping the limits of time-local approximations and guiding the design of more robust, memory-dependent closure schemes.

[1] P. Egenlauf, I. Březinová, S. Andergassen, and M. Klopotek, arXiv:2512.13913 (2025).

681	**Data-Driven Inference of Colloidal Interactions**	Florian Benedetti	Contributed talk (16:45-17:00)

Florian Benedetti (1) Tayebeh Saghaei (1) Peter D. J. van Oostrum (1) Emanuela Bianchi (2)

(1) Institute of Colloid and Biointerface Science, BOKU University, Vienna, Austria
(2) Institute for Theoretical Physics, Technische Universität Wien, Vienna, Austria

Forces between colloidal particles cannot generally be measured directly while they contribute to particle movements and ultimately drive self-assembly. We develop methods to infer the forcefield in colloidal systems from experimentally accessible trajectories. According to the Overdamped Langevin Equation (OLE) [1-2], colloidal motion is the sum of two terms: a deterministic motion caused by the total force between the colloids that depends on their (respective) coordinates and a stochastic motion due to the solvent thermal agitation, known as diffusion. Consequently, direct measurement of colloidal

motion gives only access to a noisy estimator of the total force and nothing can be said about the different components in the forcefield (i.e external field, pairwise interaction, ...). Furthermore, hydrodynamic couplings make the diffusion state dependent and the motion of one colloid becomes correlated with the motion of all the surrounding colloids [3]. Following the core idea developed in [4], we introduce a basis with physical inductive biases to capture the different phenomena behind hydrodynamic couplings. Then, using the inferred hydrodynamic couplings, we decorrelate colloidal motions and apply a similarly designed basis to disentangle the different forcefield components. Within this approach, we validate our method on both passive and active 3D systems simulated using Brownian dynamics with hydrodynamics [5]. We show that we are able to get very good quantitative agreements between the exact and inferred hydrodynamic couplings as well as the self-activity and pairwise interactions [6].

[1] I. C. Jenkins, Soft Matter, 11 (2015), 6948-6956
[2] G. Volpe, Rep. Prog. Phys., 79 (2016), 053901
[3] E. Wajnryb, Journal of Fluid Mechanics 731 (2013), 3
[4] A. Frishman, Phys. Rev. X, 10 (2020), 021009
[5] A. Callegari, F. Toschi, M. Sega, Flowing Matter. Soft and Biological Matter. Springer, Cham. (2019)
[6] F. Benedetti, In preparation

432	**Accurate Prediction of Dielectric Tensors via Equivariant Graph Neural Networks**	Erik Pabst	Contributed talk (17:00-17:15)

Erik Pabst (1) Johannes Laurenz Wolf (1) Malte Grunert (1) Max Großmann (1) Erich Runge (1)

(1) TU Ilmenau

Predicting the optical properties of solids is of great interest for a wide variety of applications, such as solar cells, optical computing and sensors. However, calculating optical properties from first principles is computationally highly demanding. Recent advances have demonstrated that graph neural networks can accurately predict the optical spectra of a wide range of materials directly from their atomic configurations. Current models, however, are predominantly centered on predicting the frequency-dependent trace of the dielectric tensor or are limited by the amount of available training data. To address these limitations, we have calculated an extensive dataset of dielectric tensors for semiconductors and insulators, consisting of over 30,000 optical spectra, using automated density functional theory calculations. Using this dataset, we trained equivariant graph neural networks, achieving excellent prediction accuracy for the full dielectric tensor.

585	**Symmetry-Aware Machine Learning for Local Structure Classification in Condensed and Soft Matter**	Jakob Hausberger	Contributed talk (17:15-17:30)

Jakob Hausberger (1) Carina Karner (1)

(1) TU Wien

Classifying local structure is a central task in condensed-matter physics and materials science. Traditional descriptors such as Steinhardt bond-orientational order parameters are widely used for this purpose, but they often struggle to distinguish structurally similar phases and perform poorly in heterogeneous or partially ordered systems. This project investigates symmetry-aware machine-learning order parameters for local structure classification as a more flexible alternative.
The proposed models operate directly on local particle neighborhoods while explicitly respecting physical symmetries such as rotation and permutation invariance. Using symmetry-aware neural architectures, including invariant encoders and autoencoders, the approach is benchmarked against classical descriptors and existing machine-learning methods on crystal and soft-matter datasets. The results show improved separation of local environments, greater robustness to disorder and interfaces, and strong potential for discovering previously unknown structural motifs. Overall, the project demonstrates that symmetry-aware machine learning provides a promising framework for physically meaningful and transferable local structure analysis.

M23 - Ab initio Modeling and Machine Learning of Crystal Defects

M23 – Session 1 (Mon 21, 10:30-12:30)			
ID	Title	Speaker	Type
58	**Machine-learning potentials for materials modeling of alloys**	Max Hodapp	Invited talk (10:30-11:00)

Max Hodapp (1)

(1) Materials Center Leoben Forschung GmbH (MCL)

In alloy modeling, atomistic simulation is a major tool that can reveal the relevant defect mechanisms influencing structural material properties (strength, fracture toughness, etc.). Traditionally, atomistic simulations have been based on empirical potentials, which, however, lack quantitative and often qualitative accuracy. For alloy screening, atomistic simulations are therefore replaced by simpler models depending only on elastic inputs (elastic constants, elastic pressure field, for instance) that can be computed with predictive electronic structure methods, such as Density Functional Theory.
In this talk, I will outline how machine-learning potentials have led to a paradigm shift that now allows for both, predicting mechanisms, and screening using defect-based models. I will then discuss training protocols for constructing machine-learning potentials that reliably predict defect properties, such as core structures, or energy barriers. Finally, I will introduce AutoPot, a software for automating such protocols requiring minimal user input.

752	**Foundational machine learning interatomic potentials: A paradigm shift in atomistic simulations?**	Matous Mrovec	Invited talk (11:00-11:30)

Matous Mrovec (1) Baptiste Bienvenu (2) Quentin Bizot (1) Anton Bochkarev (1) Ralf Drautz (1) Yury Lysogorskiy (1) Minaam Qamar (1) Sergei Starikov (1)

(1) ICAMS, Ruhr-Universität Bochum
(2) Max Planck Institute for Sustainable Materials

The emergence of foundational machine learning interatomic potentials (MLIPs) represents a transformative shift in atomistic materials simulations. These models aim to provide a scalable bridge between the predictive accuracy of first-principles methods and the temporal and spatial scales required for complex molecular dynamics simulations. Unlike traditional "bespoke" potentials tailored to specific chemical compositions or phases, foundational MLIPs are designed for universal applicability, demonstrating remarkable generalization across diverse chemical spaces and robustness in out-of-distribution environments.
This presentation focuses on the Graph Atomic Cluster Expansion (GRACE), a framework which provides a complete and efficient description of atomic interactions and unifies many current MLIP approaches. We will demonstrate the versatility of GRACE in simulations of thermodynamic, functional and mechanical properties across a broad spectrum of multicomponent systems, ranging from complex alloys to functional ceramics. Furthermore, we will critically evaluate the current issues surrounding foundation models including data quality and integrity, uncertainty quantification and strategies for ensuring reliability when moving into unknown regions of the potential energy surface, and model distillation as a path toward deriving efficient, task-specific models.

489	**Machine Learning Interatomic Potentials for Defective TaN: Balancing Energy Precision and Stress-Informed Weighting**	Kailun Sha	Contributed talk (11:30-11:45)

Kailun Sha (1) Chunhui Du (1) David Holec (2) Paul H. Mayrhofer (1) Pavel Ondračka (3) Nikola Koutná (1)

(1) TU Wien
(2) Montanuniversität Leoben
(3) Masaryk University

ransition metal nitrides (TMNs) exhibit exceptional mechanical properties influenced significantly by crystallographic defects. Modeling these defects with ab initio accuracy is challenging due to large system sizes and often lower symmetries resulting from local relaxations around a defect. In this contribution, we discuss the development of machine learning interatomic potentials (MLIPs) for cubic rocksalt TaN, targeting the impact of vacancies and deformation on potential accuracy. As a representative Group 5 system, TaN is an ideal model for investigating defect-property correlations, as its cubic phase is generally stabilized by high concentrations of vacancies on the nitrogen and tantalum sublattices.
In our work, a training and validation dataset was generated by finite-temperature ab initio molecular dynamics (AIMD) calculations, including vacancy-rich and medium-to-severely deformed supercells. While rather low precision—such as the lowest cutoff energy settings for the plane-wave basis set and only Gamma-point sampling of the reciprocal space—ensures efficient convergence, it introduces a systematic 25 GPa external pressure offset in both the Atomic Cluster Expansion (ACE, as implemented in the pacemaker package) and Moment Tensor Potentials (MTPs, as implemented in the MLIP-3 package) training frameworks. Regarding energy accuracy, both formalisms achieve a low RMSE (< 9 meV/atom), with ACE exhibiting superior performance (< 2 meV/atom). However, MTP-type force fields offer a distinct advantage for mechanical modeling; their training framework allows for explicit stress weighting in the loss function, capturing elastic responses often overlooked in pure energy fitting.
Finally, large-scale molecular dynamics (MD) simulations reveal a vacancy-induced phase transition from the rocksalt structure to a hexagonal-like system. These results underscore the necessity of balancing energy precision with stress-informed weighting to accurately predict the stability and mechanical behavior of defective TMNs.

422	**Capturing step-flow growth and defect formation in silicon carbide combining molecular dynamics and Monte Carlo simulations**	Alexander Reichmann	Contributed talk (11:45-12:00)

Alexander Reichmann (1) Zahra Rajabzadeh (1) Lorenz Romaner (1)

(1) Montanuniversität Leoben

Simulations of SiC crystal growth on an atomistic scale were, in the past, most commonly done with Monte Carlo (MC) based methods, such as kinetic lattice MC or kinetic super lattice MC. These, however, suffer from the fact that they have to use predefined deposition sites and reaction rates, making it difficult to realistically simulate defects, such as dislocations or stacking faults. With the rise of accurate interatomic potentials, MD simulations of SiC

crystal growth have also been conducted. These, however, have the shortcoming of too small simulation times, therefore needing to use growth rates which are ~108 times larger than real-life SiC growth rates. A recently developed method, called the Minimal Energy Atomic Deposition (MEAD), combines both MD and MC and tries to seamlessly overcome both of these simulation hurdles.
The MEAD algorithm works by first scanning the surface of the substrate for deposition sites with low potential energy. Then these deposition sites are populated by either Si or C atoms. After this deposition step, temperature is applied to the system by using time-stamped force-biased MC (tfMC). This allows the system to get into equilibrium and for the deposited atoms to reach their minimum energy position at the required temperature. This three-step process of scanning the surface for potential deposition sites, then populating the lowest ones and applying temperature to the system, is then repeated until sufficient growth has been simulated.
In this talk, we will present our effort of applying the MEAD simulation method to the SiC system. We apply different temperatures ranging from 2300 to 2500 K and identify the polytypes grown, using this method on both the C-terminated and Si-terminated 4H SiC surface. In addition, defects, vacancies and add-atoms occurring during growth will be investigated, as well as growth on stepped surfaces. We also compare different interatomic potentials in terms of their predicted SiC growth structure. In this way, we hope to gain new insights into the atomistic mechanisms governing the growth process of SiC.

120	**First-principle based description of defects in complex alloys with magnetic and compositional disorder**	Franco Moitzi	Contributed talk (12:00-12:15)

Franco Moitzi (1) Philipp Hammer (1) Max Hodapp (1) Oleg Peil (1) Vsevolod Razumovskiy (1) Andrei Ruban (1)

(1) Materials Center Leoben Forschung GmbH

Most metallic alloys of technological relevance, such as steels and superalloys, are inherently complex due to the coexistence of chemical disorder and, in many cases, magnetic disorder. This is particularly important in Fe-based systems, where the magnetic state can vary with temperature and composition. Capturing these effects within first-principles approaches remains challenging, especially when extended defects such as dislocations, stacking faults, and interfaces are involved.
In this work, we focus on impurity–defect interactions in Fe-based systems across different crystal structures, magnetic states, and defect types. We employ a combination of advanced computational methods, including Green's-function-based density functional theory and machine-learning(ML)-assisted approaches, such as actively learned interatomic potentials, to study how alloying and magnetic disorder influence defect properties. The former offers a particular advantage in that chemical and magnetic disorder can be treated consistently and efficiently within a single unified framework, namely the coherent potential approximation together with the disordered local moment model, making the approach efficient. The ML methods are applied in specific regimes where their scalability provides clear benefits.
The results indicate that magnetic effects play a central role in determining segregation tendencies and defect-solute interaction energies, often exceeding contributions from purely elastic size mismatch. In addition, these interactions are found to depend sensitively on the magnetic state, temperature, and thermal vibrations.
Overall, the study highlights the importance of consistently accounting for the correct magnetic state and disorder when describing defects in alloys.

405	**Magnetic exchange interactions at grain boundaries in iron**	Martin Zelený	Contributed talk (12:15-12:30)

Martin Zelený (1) Martin Heczko (2) Petr Šesták (1) Denis Ledue (3) Renaud Patte (3) Miroslav Černý (1)

(1) Faculty of Mechanical Engineering, Brno University of Technology
(2) Faculty of Metals Engineering and Industrial Computer Science, AGH University of Krakow
(3) Normandie Université, UNIROUEN, INSA Rouen

Grain boundaries (GBs) play an important role in polycrystalline magnetic materials because they act as obstacles to magnetic domain wall motion. Therefore, magnetic coercivity, remanence, saturation magnetization, and the Curie temperature are known to depend strongly on grain size. An atomistic description of magnetic interactions requires construction of an effective Heisenberg Hamiltonian containing exchange interaction parameters J_{ij} between pairs of atomic sites. The values of J_{ij} can be obtained from ab initio calculations. Knowledge of these parameters further enables simulations of larger systems and/or excited states at nonzero temperatures using Monte Carlo techniques. Information about J_{ij} is available in the literature for many bulk magnetic materials. However, so far there has been no information about J_{ij} in the vicinity of GBs, where the symmetry of the crystal lattice is reduced and atoms have a different chemical environment.
In the present work, we provide a detailed analysis of J_{ij} obtained from ab initio calculations in the vicinity of a clean Σ5(310) GB in bcc Fe, as well as of a GB with segregated P impurities. Negative J_{ij} values were found for interactions across the clean GB, indicating a preferred antiferromagnetic alignment of magnetic moments on these atoms. This demonstrates the strong influence of the GB on exchange interactions in Fe. Monte Carlo results show that, despite pronounced local perturbations, realistic GB densities cause only a small reduction in the Curie temperature because bulk-like regions dominate the global magnetic transition. A substantial decrease in the Curie temperature appears only when the GB volume fraction is artificially increased.

M23 – Session 2 (Tue 22, 10:30-12:45)			
ID	Title	Speaker	Type
328	**Vacancy-Controlled Strengthening and Toughening Mechanisms in Transition Metal Nitrides**	David Holec	Invited talk (10:30-11:00)

Rui Zhang (1) Kan Zhang (2) David Holec (1)

(1) Montanuniversität Leoben
(2) Jilin University

Transition metal nitrides (TMNs) are vital protective coatings for structural and moving components due to their exceptional thermal stability, corrosion resistance, and mechanical properties. However, their strong covalent/ionic bonding and limited slip systems often lead to brittle fracture. Recent studies suggest that defect engineering—specifically via vacancies—is a promising strategy to achieve a synergy of strength and toughness. Despite this potential, the specific influence of different metal species and vacancy configurations on the mechanical response remains poorly understood. In this work, we systematically investigate IIIB-VIB group binary nitrides by introducing 10% and 20% concentrations of nitrogen and metal sub-lattice vacancies. Utilizing the high-fidelity GRACE universal potential, we performed shear simulations to compare strain behaviors and structural responses at 0K and 300K. Our results elucidate how metal species and vacancy configurations dictate the shear strength, deformation pathways, and maximum strain capacity of TMNs. This study clarifies the mechanisms of vacancy-driven strengthening and toughening, providing a theoretical foundation for the targeted design of high-performance ceramics.

718	**Defect-Engineered Ferroelectricity and Magnetoelectric Coupling in $LaXO_3$ Perovskite Oxides**	Souren Majani	Contributed talk (11:00-11:15)

Souren Majani (1) Ulrich Aschauer (1)

(1) Paris Lodron University of Salzburg

Ferroelectricity, a key functional property for non-volatile memory, sensors, actuators, and low-power electronic devices, can emerge through several microscopic mechanisms. Conventional ferroelectricity in oxide perovskites is often associated with second-order Jahn–Teller distortions involving empty d-orbital transition-metal cations, while alternative routes such as epitaxial strain, improper ferroelectricity, charge ordering, lone-pair activity, and defect-induced symmetry breaking provide additional pathways toward polar order. However, achieving robust ferroelectricity in magnetic oxides remains challenging because the electronic configurations that favor magnetism often suppress the conventional polar instability. Single-phase materials that combine switchable polarization and magnetic order, particularly near or above room temperature, therefore remain a major target in the design of multifunctional oxides.
Here, we propose a systematic first-principles investigation of defect-induced ferroelectricity in the $LaXO_3$ perovskite family, where X represents a transition-metal cation such as V, Cr, Mn, Fe, Co, or Ni. Building on the antisite-defect mechanism identified in $LaFeO_3$, we examine whether transition-metal antisites can locally break inversion symmetry and stabilize polar structures across chemically distinct $LaXO_3$ compounds. Density functional theory calculations are employed to evaluate defect formation energetics, relaxed atomic distortions, polarization, electronic structure, magnetic ordering, and switching pathways. By analyzing the interplay between crystallographic symmetry, A/B-site ionic size mismatch, octahedral distortion modes, and magnetic ordering, this study establishes a framework for understanding and tuning the emergence of coupled ferroic functionalities in defect-engineered $LaXO_3$ perovskite oxides. Ultimately, this study emphasizes the significance of defect engineering as a powerful tool for rational material design and optimization.

487	**Segregation of vacancies to grain-boundaries in W**	Christoph Dösinger	Contributed talk (11:15-11:30)

Christoph Dösinger (1) Oliver Renk (1) Lorenz Romaner (1)

(1) Montanuniversität Leoben

Both vacancies and grain-boundaries (GB) are important defects in materials. The vacancies can interact with the GBs which might lead to a formation of voids, as a result this might start the formation of pores or cracks. From atomistic simulations it is known, that vacancies can be attracted to GBs, which indeed may act as sinks for the vacancies. In this work we use ab-initio methods to study the attraction of vacancies to GBs in tungsten. This is done via calculating the segregation energy that quantifies a defect's attraction towards GBs. In the study we include 15 different coincident site lattice GBs ranging from $\Sigma 3$ to $\Sigma 43$ enabling a representative overview of segregation behaviours. In addition to the segregation energies also structural changes of the GB are observed which are characterized by a change of the stress-state of the atomistic structure and the width of the GB. Combining these results allows to estimate overall size-changes due to annealing of vacancies at GB in nano-crystalline materials produced using e.g. high pressure torsion. The results show a few segregation sites towards which the vacancies are strongly attracted, where the segregation energy corresponds to the vacancy formation. Relaxation of the atomistic structure leads to a filling of the vacancy which is accompanied by reduction of the GB width. However, the majority of sites show intermediate segregation energies, where the vacancy remains stable, i.e. is not filled.

407	**Doping of tin sulfide for novel phase stabilisation**	Guy Makov	Contributed talk (11:30-11:45)

Yuval Golan (1) Guy Makov (1) Neeraj Mishra (2) Susmita Paul (1)

(1) Ben-Gurion University
(2) University of Alberta

Tin based monchalcogenides are environmentally attractive alternative to the well known lead based monochalcogenides in thermoelectric and electrooptical applications. Specifically, the novel cubic phase of tin monosulphide, π-SnS, is of significant interest due to its attractive material properties, such as a wider band gap suitable for solar photovoltaic application and relative ease of epitaxial deposition onto technologically relevant semiconductors compared to the thermodynamically stable orthorhombic phase of α-SnS. However, this phase is thermodynamically metastable and experimentally restricted to the nanometric scale. We explore computationally and experimentally the effect of introducing doping on stabilizing phases, and show that introducing Pb impurities improves phase stability of π-SnS over α-SnS. However, replacing Pb2+ with alternative non-toxic, environmentally friendly cations

for cubic phase stabilization would be clearly advantageous. We have computationally investigated the energetics and electronic properties of calcium ion impurities in both SnS polymorphs.Computational results indicated that ~11 cat% of Ca2+ ions are required for preferred growth of π-SnS over α-SnS. We confirmed experimentally that addition of Ca2+ cations enables phase control of SnS grown from solution from α-SnS to π-SnS, forming compact films of π-SnS. Furthermore, the presence of an intermediate layer of CaS is computationally predicted to significantly contribute to the stabilization of the π-SnS phase, thereby reducing the Ca concentration required, which aligns well with experimental observations. Subsequently, we find that CaS is a promising substrate for epitaxial growth of π-SnS in the (111) orientation. Moreover, the bandgap of π-SnS decreased only slightly with increasing concentration of Ca cations in the material. These results can facilitate the bulk scale synthesis of π-SnS material, bringing it closer to practical utility for a range of applications.

428	**Spin-Selective Optical Cycles in Color Centers**	Mirjam Neubauer	Contributed talk (11:45-12:00)

Mirjam Neubauer (1) Maximilian Schober (1) Michel Bockstedte (1)

(1) Institute for theoretical Physics, Johannis Kepler University Linz

Prototypical Color Centers in semiconductors, such as the NV^--center in diamond, the Silicon vacancy (V_{Si}^-) and the di-vacancy ($V_C V_{Si}$) in 4H-Silicon carbide (4H-SiC) are promising candidates for the implementation of quantum bits (qubits) in semiconductors. Their coupled electron spins exhibit correlated high- and low-spin states, enabling spin-selective manipulation via optical excitation, magnetic fields or strain. Optical spin manipulation involves excitations within the high-spin multiplet and spin-selective non-radiative transitions (intersystem-crossing, ISC), mediated by spin-orbit, spin-spin, and electron-phonon interactions. Together with the zero-field splitting in ground and excited states, these processes enable diverse spin-photon protocols. A quantitative understanding of spin-selective interactions is essential for optimizing such quantum interfaces. We describe Color Centers using an embedding approach based on a configuration-interaction (CI) Hamiltonian with an effective screened Coulomb interaction [1,2], extended by a perturbative treatment of the spin-orbit coupling [3]. In combination with the electron-phonon coupling this framework provides access to spin-selective transition rates and photo ionization [3,4]. We demonstrate the approach by analyzing the spin-selective optical cycle of the V_{Si}^- in 4H-SiC. Our results yield a quantitative understanding of the underlying processes and open the door to theory-guided qubit engineering.

[1] M. Bockstedte et al., npj Quantum Materials 3, 31 (2018).
[2] M. Niethammer et al., Nano Letter 19, 7173 (2019).
[3] M. Neubauer et al., Key Eng. Mat. 984, 1 (2023).
[4] T. Steidl et al., Nat. Commun. 16, 4669 (2025).

121	**Ab initio modeling of mechanical properties in Fe-Si-Al alloys using Machine Learned Interatomic Potentials**	Daniil Khodachenko	Contributed talk (12:00-12:15)

Daniil Khodachenko (1,2) Max Hodapp (1) Oleg Peil (1) Vsevolod Razumovskiy (1)

(1) Materials Center Leoben Research GmbH
(2) Christian Doppler Laboratory DMDG-MAE

Unique electromagnetic properties of steels with silicon and aluminum make them an excellent choice for the production of transformers and electric motors. These so-called electrical steels have enhanced energy efficiency due to reduced core losses and enhanced magnetic permeability. However, increasing the concentration of silicon and aluminum beyond a critical amount leads to significantly reduced ductility, which makes production very challenging.
The origins of these embrittlement effects from a first-principles perspective are still not fully understood, as ab initio modeling based on conventional Density Functional Theory (DFT) is computationally very expensive, due to the requirement of large supercells, for the treatment of disorder, and complex magnetic interactions. While bulk configurations can also be described by the Coherent Potential Approximation (CPA), real systems are never perfectly symmetric crystals, where in particular planar defects such as stacking faults are known to have a significant impact on mechanical properties of materials. However, accuracy comparable to DFT can be achieved through the application of Machine Learned Interatomic Potentials (MLIPs). Using the recently developed workflow manager Autopot [1] we train Moment Tensor Potentials (MTPs) for the Fe-rich region of the ternary Fe-Si-Al system, containing both bulk configurations, and configurations containing a stacking fault. This potential is then used to predict properties relevant for the study of dislocation plasticity, namely lattice constants, elastic constants, and unstable stacking faults. Our work shows that an MTP-based workflow of this kind can pave the way for the description of failure mechanisms in multicomponent alloys.

350	**Atomistic description of crystal defects in SiC**	Lorenz Romaner	Contributed talk (12:15-12:30)

Lorenz Romaner (1) Georg Holub (1) Celine Halkali (1) Zahra Rajabzadeh (1)

(1) Montanuniversität Leoben

Silicon carbide (SiC) is a wide-band semiconductor with exceptional properties for applications in power electronics. It outperforms Si as a semiconductor in terms of electric breakdown field, saturation carrier velocities and thermal conductivities. Especially the latter makes SiC also more attractive compared to other wide band semiconductors such as GaN. In general, crystal defects play a central role for electric and optical properties and deep atomistic insights are still missing.
In this talk we present calculations including densitiy functional theory and interatomic potentials to explore the properties of crystal defects in SiC. We focus on the energetics of polytypes, point defects, dopants, dislocations, grain boundaries and surfaces. With respect to dislocations we show the core structure of SiC and explore the formation of hollow micropipes as a function of Burgers vector size. We find that commonly observed inner radii are smaller in theory compared to experiments and discuss the possible reasons for the discrepancy. Furthermore, we discuss point defects in SiC that are relevant for quantum sensing applications. We investigate the relevant defect levels and study their properties in different crystallographic environments. Finally we also present out activities to develop machine learning interatomic potentials that can be used to explore deposition phenomena of crystal growth that are relevant crystal growth to understand how the quality of SiC crystals can be improved during the physical vapor transport process.

746	**Efficient descriptors for modeling of disordered metallic alloys**	Oleg Peil	Contributed talk (12:30-12:45)

Oleg Peil (1)

(1) Materials Center Leoben Forschung GmbH, Leoben, Austria

Description of disordered alloys from first principles has always been a challenge. The rise of machine learning (ML) methods has opened new opportunities in this endeavor, but thus far, most of data-driven approaches treat alloys as yet another atomistic system, disregarding important properties of solid solutions, such as homogeneity and translational invariance on average. At the same time, mean-field methods, such as coherent potential approximation, can provide a very reasonable representation of an idealized alloy system, however they fail at capturing deviations from the ideal homogeneous state, which is often the case at or near to crystal defects. In this work, we present how alloy models of various levels of complexity could be combined to improve efficiency of ML methods in applications to disorder alloys. Examples of applications to high entropy alloys will be demonstrated, which includes Fe-group alloys, whose magnetic behavior makes their description even more challenging.

M23 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
65 **P023**	**Exploring Magnetism, Half-Metallicity, and Thermoelectric Response in Antifluorite-Type K_2IrX_6 (X = Cl, Br, and I) Hexahalides: A First-Principles Study**	Asma Bouabca	Poster

Asma Bouabca (1) Habib Rozale (2)

(1) Wave and Acoustic Laboratory (LPM), Physics Faculty, USTHB, Algeirs, Algeria
(2) Condensed Matter and Sustainable Development Laboratory (LMCDD), University of Sidi Bel-Abbes, Sidi Bel-Abbes, 22000, Algeria

In this work, we present a comparative first principles study of the cubic K_2IrX_6 (X = Cl, Br, I) halides, focusing on their structural, mechanical, electronic, magnetic, thermodynamic, and thermoelectric transport properties. Structural optimization confirms mechanical stability for all compounds, and reveals a systematic increase in lattice constant and unit cell volume from Cl to I, consistent with the larger halogen ionic radii. Spin polarized electronic calculations show strong spin asymmetry near the Fermi level, with a metallic majority spin channel and a minority spin gap that narrows along the series, reflecting enhanced Ir-X hybridization. The total and projected density of states indicate that Ir 5d and halogen-p states dominate the electronic activity around EF, while potassium contributes negligibly. Thermodynamic properties evaluated using the quasi-harmonic Debye model exhibit physically consistent temperature and pressure dependent trends for Gibbs free energy, entropy, thermal expansion, volume, and Debye temperature. Boltzmann transport calculations predict pronounced temperature dependence of the Seebeck coefficient and electrical conductivity, and the resulting thermoelectric figure of merit increases across the series, reaching its highest value for K2IrI6 due to the combined balance between the power factor and reduced lattice thermal conductivity. Overall, the K_2IrI_6 family emerges as a mechanically stable and electronically tunable platform with promising multifunctional behavior relevant to electronic and energy related applications.

468 **P024**	**Phase-dependent shear behaviour in MAB phases driven by Al layers and defects using ML potentials**	Priyanshu Sorout	Poster

Priyanshu Sorout (1) Shuyao Lin (1,2) Paul H. Mayrhofer (1) Davide G. Sangiovanni (2) Nikola Koutná (1,2)

(1) Institute of Materials Science and Technology, TU Wien, Vienna, Austria
(2) Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Layered transition-metal aluminum borides (MAB phases) are promising for high-temperature applications, combining ceramic-like oxidation resistance with metal-like fracture toughness by incorporating compliant Al layers within the MBene structure. Although their tensile properties have been extensively studied, shear deformation, especially relevant given their layered yet puckered architecture, remains largely unexplored. To address this gap, using purpose-trained ML potentials, we systematically investigate atomic and nanoscale finite-temperature shear deformation up to 10,000 atoms in MAB phases across Group IV-VI transition metals. We focus on three representative polymorphs: 212-, 222-, and 314-type. Our results reveal strongly phase-dependent ideal shear strengths, ranging from 10 GPa to 25 GPa across nine compositions. We find that mechanical instability is initiated by the gliding Al interlayer, which serves as the preferred slip plane due to the relatively weak, metallic Ti-Al bonding compared to the covalent B-Ti framework. Furthermore, introducing Al vacancies reduces the ideal shear strength and facilitates interlayer sliding, highlighting vacancy concentration as a key parameter for layer separation into MBenes. Altogether, this study establishes Al-layer-driven shear behaviour in MAB phases as a function of structural polymorph and point defects, using reliable machine-learning potentials, and provides guidance for the synthesis of future two-dimensional materials.

M24 - Computational Frontiers in Structure Prediction, Lattice Dynamics, and Electron-Phonon Coupling

M24 – Session 1 (Thu 24, 16:00-18:00)			
ID	Title	Speaker	Type
104	**Structural disorder and superconductivity: what first-principles calculations can already tell us**	Simone Di Cataldo	Invited talk (16:00-16:30)

Simone Di Cataldo (1) Lilia Boeri (1) Alessio Cucciari (1)

(1) Sapienza University of Rome

Real-space disorder through interstitial impurities, substitutional alloying, or vacancy ordering, is rarely treated on equal footing with the ideal crystal in ab initio studies of superconductivity. Yet the tools to do so exist: supercell-based electron-phonon calculations have reached a level of maturity where quantitative predictions for disordered systems are within reach, even at moderate computational cost [1-3].
In this talk, I will discuss what can already be learned from this approach, despite the inherent limitations in supercell size. Through examples spanning interstitially doped aluminum, transition-metal alloys, and carbides with vacancies, I will show that real-space disorder can modify superconducting properties through qualitatively distinct channels: phonon softening or local changes in electron-phonon matrix elements. I will argue that coupling is way more sensitive than the overall electronic disorder. with effects ranging from detrimental to strongly beneficial.

[1] PN Ferreira et al., Materials Today Physics 48, 101547, 2024
[2] A. Cucciari et al., Phys. Rev. B 110, L140502, 2024
[3] S. Di Cataldo et al., npj Computational Materials 12, 73 2026

216	**Toward a predictive ab initio description of superconductivity in NbN**	Eva Kogler	Invited talk (16:30-17:00)

Eva Kogler (1) Peter I. C. Cooke (2) Christoph Heil (1) Mahmoud I. Hussein (3,4) Matthew N. Julian (5) Fabian Jöbstl (6) Birgit Kunert (7) Roman Lucrezi (8) Chris J. Pickard (2) Rohit Prasankumar (5) Roland Resel (7) Mihir Sahoo (1) Chia-Nien Tsai (3)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology
(2) University of Cambridge
(3) Smead Department of Aerospace Engineering Sciences, University of Colorado, Boulder
(4) Department of Physics, University of Colorado, Boulder
(5) Enterprise Science Fund, Intellectual Ventures, Bellevue, Washington
(6) Universität Wien
(7) Institute of Solid State Physics, Graz University of Technology
(8) Department of Chemistry, Stockholm University,

NbN is a workhorse superconductor in quantum devices, detectors, and high-field applications, yet a quantitative microscopic description of its structure and superconducting behavior remains incomplete. Predictions of the critical temperature (T_c) are systematically higher than experimental values, indicating missing ingredients in current models. Open questions remain regarding the role of nitrogen vacancies, disorder, low dimensionality, and anharmonicity, and how these factors influence stability, the Eliashberg spectral function $\alpha^2F(\omega)$, and ultimately T_c. Addressing these challenges requires going beyond state-of-the-art approaches, including the use of machine learning potentials to overcome computational limitations.
By examining how subtle structural and dynamical effects shape superconducting properties, this work on NbN bridges first-principles calculations with experimental observables and enables a predictive framework for related superconducting materials.

380	**Escaping Local Minima: Searches for Ternary Hydride Superconductors Using hot-AIRSS**	Kieran Bozier	Contributed talk (17:00-17:15)

Kieran Bozier (1) Maélie Caussé (1bridge) Peter I.C. Cooke (1) William Galloway (1) Johannes Meusburger (1) Chris J. Pickard (1) Stefano Racioppi (1)

(1) University of Cambridge

The search for novel conventional superconductors is increasingly turning towards ternary and quaternary systems with large unit cells. However, because the number of local minima scales exponentially with the number of atoms, purely DFT-driven crystal structure prediction struggles to explore these complex energy landscapes and reliably determine thermodynamic stability. To address this challenge, we employ the recently developed hot-AIRSS methodology [1]. By leveraging machine-learned interatomic potentials to perform short molecular dynamics runs between structural relaxations, this approach greatly accelerates investigations of these larger cells. We apply this workflow to search for promising ternary hydrides at 100 GPa, coupling the hot-AIRSS search with high-throughput electron-phonon coupling calculations - accelerated by up to two orders of magnitude via density of states rescaling [2] - to solve the Eliashberg equations for the superconducting transition temperature. We will present the results of this search, discussing the structural diversity, thermodynamic stability, and predicted T_c values of the most promising candidate phases.

[1] CJ Pickard. “Beyond theory-driven discovery: introducing hot random search and datum-derived structures”. In: Faraday Discussions 256.0(2025), pp. 61–84.
[2] K Bozier et al. “High-throughput superconducting Tc predictions through density of states rescaling”. In: Physical Review B 113.6 (2026), p. 064507.

692	**Comprehensive First-Principles Description of Spin–Phonon Coupling in Nitrogen–Vacancy Diamond**	Zhishuo Huang	Contributed talk (17:15-17:30)

Zhishuo Huang (1) Ruben Baumgarten (1y) Priyamvada Jadaun (1)

(1) Electrical Engineering and Computer Science, Technische Universität Berlin, 13355 Berlin, Germany

The nitrogen–vacancy (NV) centre in diamond is a leading platform for nanoscale quantum sensing of magnetic fields, temperature, and strain. Sensing sensitivity is fundamentally bounded by the spin–lattice relaxation time T_1, making its accurate prediction essential for optimizing quantum sensor performance. Cambria et al.[1] advanced this goal with an ab initio framework reproducing NV relaxation rates from 9–474 K and identifying second-order spin–phonon processes as the dominant Raman mechanism. However, their Γ-point Brillouin-zone sampling in a finite supercell leaves the continuous phonon dispersion unresolved, likely causing the reported eightfold underestimation of the single-quantum relaxation rate. More broadly, no existing treatment consistently couples correlated wavefunction methods for the defect's multi-reference electronic structure with rigorous periodic lattice dynamics for the host crystal[2].
We present a framework that closes this gap. Quantum chemistry calculations on embedded NV clusters yield spin-state-resolved energies and spin–orbit coupling derivatives with high-level electron correlation, while density functional perturbation theory within Quantum ESPRESSO[3] provides the full phonon dispersion across the Brillouin zone. These are connected via Wannier-interpolated electron–phonon matrix elements (EPW)[4] on dense wavevector grids. The resulting spin–phonon coupling Hamiltonian enables parameter-free evaluation of T_1, resolving direct, Raman, and Orbach processes over the full temperature range, and identifies which phonon branches and Brillouin-zone regions dominate relaxation at each temperature. This provides a microscopic basis for phonon engineering strategies transferable to other solid-state spin defect platforms, opening pathways for enhancing T_1.

[1] M.C. Cambria et al., PRL 130, 256903 (2023).
[2] M. Onizhuk, G. Galli, RMP 97, 021001 (2025).
[3] P. Giannozzi et al., JPCM 21, 395502 (2009).
[4] S. Poncé et al., CPC 209, 116 (2016).

711	**Challenges in Machine-learning Based Non-Adiabatic Molecular Dynamics for Nano-porous Graphene**	Bernhard Kretz	Contributed talk (17:30-17:45)

Bernhard Kretz (1) Ivor Loncaric (1)

(1) Institut Rudjer Boskovic

Nano-porous graphene (NPG) offers great potential across a range of applications, from electronics to photocatalysis. Its electronic properties, e.g., the band gap, can be tuned by changing structural parameters alone[1]. In order to optimize NPG for photo-physical and photo-chemical applications, their excited-state properties need to be studied. The method of choice for studying dynamic excited-state properties is often non-adiabatic molecular dynamics (NAMD). However, conventional NAMD relying on ab-inito methods to describe ground- and excited-state potential energy surfaces is computationally expensive, particularly for periodic systems. Employing machine-learning methods can significantly reduce the computational cost of NAMD without compromising accuracy [2], but may come with their own challenges for periodic systems.
In our work, we trained machine-learning interatomic potentials for the ground state and the five lowest excited singlet states for a specific NPG. We used these potentials in combination with Landau-Zener surface hopping [3] to run NAMD simulations for the NPG. Our findings show that the number of excited states included in the NAMD simulations affects the relaxation to the ground state. Furthermore, our NAMD simulations reveal the limitations of the chosen approach to NAMD simulations for periodic systems. In this contribution, we will discuss the advantages of the approach employed in this work as well as its limitations.

[1] (a) F. Crasto de Lima, A. Fazzio, Phys. Chem. Chem. Phys. 23 (2021) 11501-11506; (b) D. Wang, X. Lu, Arramel, M. Yang, J. Wu, A. T. S. Wee, Small 17 (2021) 2102246; (c) B. Kretz, I. Lončarić, Inorg. Chem. 64 (2025) 11022-11031.
[2] J. Li, S. A. Lopez, Chem. Phys. Rev. 4 (2023) 031309
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477	**Understanding How Pressure Enhances Heat Transport in Organic Semiconductors**	Lukas Legenstein	Contributed talk (17:45-18:00)

Lukas Legenstein (1) Sandro Wieser (2) Michele Simoncelli (3) Egbert Zojer (4)

(1) Montanuniversität Leoben, Graz University of Technology
(2) TU Wien
(3) Columbia University, NY
(4) Graz University of Technology

Understanding how lattice thermal conductivity changes under strain or pressure is increasingly important in materials science, yet difficult to predict because a material's behavior can range from monotonic increases or decreases to anomalous trends. Molecular crystals, including organic semiconductors, stand out for exhibiting unusually large pressure-induced increases relative to their (ultra-)low thermal conductivities. However, the atomistic mechanisms underlying these significant pressure enhancements have yet to be elucidated.
Our test system, naphthalene, crystallizes in a herringbone packing motif common in most π-conjugated organic semiconductors which is strongly affected by external pressure. Measurements up to 2 GPa from previous literature show an isotropic thermal conductivity that is up to four times higher than at ambient conditions. By combining highly accurate machine-learned potentials with the Wigner transport equation, we not only reproduce these findings but also elucidate how compression affects naphthalene's anisotropic thermal conductivity and how phonon tunneling becomes less relevant with increasing pressure. Finally, we trace the pressure-induced enhancement to frequency upshifts and the associated modifications in phonon scattering.

M24 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
56 **P049**	**Ab initio excitons and electron-phonon coupling in half-Heuslers**	Vinod Solet	Poster

Vinod Kumar Solet (1) Sudhir K. Pandey (1)

(1) Indian Institute of Technology Mandi, Himachal Pradesh, India

This Half-Heusler compounds are currently considered promising photovoltaic (PV) and thermoelectric (TE) materials owing to their favorable electronic, optical, thermopower and electrical conductivity properties. Using first-principles density-functional theory (DFT) and many-body–based methods such as the GW approximation, Bethe–Salpeter equation (BSE), and electron–phonon interactions (EPI) [1, 2], we study the quasiparticle band structures, optical excitonic properties, and charge mobility of LiZnAs and ScAgC. These materials direct-band-gap semiconductors and both exhibit triply degenerate, loosely bound bright excitons (with binding energies in the range of 45–55 meV) at the main absorption peak 1. Furthermore, these excitons are highly localized (delocalized) in momentum (real) space, indicating the presence of Mott–Wannier–type excitons at the band gap 1. Next, the temperature-induced renormalization of the electronic states due to EPI is obtained within the non-adiabatic Allen–Heine–Cardona formalism 2. We then solve the Boltzmann transport equation (BTE), both iteratively and within multiple relaxation-time approximations (RTAs), to evaluate the carrier transport. Phonon-limited electron and hole mobilities computed using the linearized self-energy and momentum RTAs (SERTA and MRTA) are compared with the iterative BTE (IBTE) results 2. Finally, we obtain a spectroscopic limited maximum efficiency (SLME) in the range of ~31–32% at a thin-film thickness of ~0.4 μm 1, and a TE figure of merit (zT) in the range of ~0.8–1.0 (for bulk) and ~1–1.5 (for nanostructured samples) 2. These findings highlight the significant role of excitons in the solar energy absorption process and electron–phonon coupling in charge transport, and also suggest that both materials are highly suitable candidates for next-generation single-junction thin-film PV solar and TE devices.

(1) V. K. Solet and S. K. Pandey, Phys. Rev. Appl. 23, 064040 (2025).
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415 **P050**	**Reliable Super-Resolution for Real-Time Electronic Structure Theory**	Alexander Gorfer	Poster

Alexander Gorfer (1) Matthias Kick (1) Karsten Reuter (1)

(1) Fritz Haber Institute of the Max Planck Society, Berlin, Germany

Calculating excited state spectra of large systems is often prohibitively expensive with standard frequency-domain methods such as the Casida equations, the Bethe-Salpeter Equation (BSE), or Equation-of-Motion Coupled Cluster (EOM-CC). Real-time methods provide an alternative, as all modes are excited simultaneously. However, long simulation times are required to resolve narrow spectral features with traditional Fourier signal analysis, significantly limiting system size. Super-resolution methods such as Compressed Sensing promise high-resolution spectra from much shorter signals but assume the spectrum to be sparse, an assumption which breaks down in larger systems where sharp features are embedded in a quasi-continuum of smaller nearby peaks. To overcome this, we combine newly designed highly noise-tolerant super-resolution techniques with physically motivated filtering. Using approximate frequency information, we identify the brightest transitions and extract only these important modes from the time propagation. By doing so, we effectively precondition the problem for super-resolution, reducing the number of required time steps for signal reconstruction to a minimum. We demonstrate our approach on systems containing several hundred heavy atoms, achieving up to 20-fold speedups while maintaining spectral accuracy even for signals dominated by large continua.

421 **P051**	**Universal MLIPs for High-Throughput Anharmonic Stability Screening**	Ralf Meyer	Poster

Ralf Meyer (1) Christoph Heil (1)

(1) Institute of Theoretical and Computational Physics, Graz University of Technology

Computational high-throughput screening for superconducting materials relies critically on the accurate assessment of dynamical stability. Systems with strong electron-phonon coupling are among the most promising candidates for high-temperature superconductivity, but are also precisely those most prone to lattice instabilities, including metastable phases such as hydrides at elevated pressures. Anharmonic effects are particularly significant in these and other light-element or structurally complex compounds, where harmonic approximations routinely fail to capture the true lattice behavior. The stochastic self-consistent harmonic approximation (SSCHA) represents an accurate method to capture these effects, but its combination with density functional theory (DFT) carries a substantial computational cost, rendering large-scale screening intractable in most settings.
Recently proposed workflows have addressed this bottleneck by employing system-specific machine-learning interatomic potentials (MLIPs) trained for individual systems, significantly reducing the computational burden while retaining DFT-level accuracy. In this work, we explore whether universal MLIPs (uMLIPs), trained across broad chemical spaces, can achieve comparable accuracy without the overhead of system-specific training. This can further lower the barrier to large-scale deployment and enable exploration of design spaces previously excluded based on harmonic stability analysis. We benchmark the uMLIP-based approach across a set of representative systems and discuss the feasibility of integrating anharmonic stability analysis into high-throughput screening workflows.

425 **P052**	**Machine Learning of Temperature-Dependent Optical Spectra**	Johannes Laurenz Wolf	Poster

Johannes Laurenz Wolf (1) Erik Pabst (1) Malte Grunert (1) Max Großmann (1) Erich Runge (1)

(1) TU Ilmenau

Recent advances have demonstrated that neural networks can accurately predict optical spectra of a wide range of materials directly from atomic configurations. However, most existing approaches are limited to equilibrium structures at 0 K and therefore fail to capture temperature-dependent effects. Modeling such effects requires accounting for electron–phonon interactions, which is computationally demanding due to the need for extensive sampling of

thermally perturbed configurations or explicit first-principles phonon calculations. Accurate temperature-dependent optical spectra are, however, crucial for applications such as photovoltaics and optoelectronic devices, where material performance is strongly influenced by thermal effects under operating conditions.
In this work, we present a computational framework that utilizes machine learning interatomic potentials to efficiently generate large ensembles of thermally perturbed atomic configurations via molecular Dynamics simulations. These configurations are combined with density functional theory (DFT) calculations to produce reference optical spectra, which are then used to train a neural network model. This approach enables the prediction of temperature-dependent optical spectra with accuracy comparable to the underlying DFT calculations at a fraction of the computational cost.
We demonstrate the performance of our method on III–V semiconductors, showing that the neural network captures the temperature response of optical spectra even when trained on limited data. Our framework provides a scalable pathway for studying finite-temperature optical properties and significantly accelerates the exploration of thermally driven phenomena in materials.

649 **P053**	**Predicting Oxygen-Centered Polarons From Local Disorder in NMC622**	Cristian Vijeu	Poster

Maria Alfredsson (1) Furio Cora (2) Cristian Vijeu (1)

(1) University of Kent
(2) University College London

Reliable structural prediction in functional materials requires atomistic models that capture both the intended cation arrangement and the local disorder that control electronic behaviour. In this work, we study layered NMC622 using spin-polarized DFT simulations. The simulated cation ordering is benchmarked against experimental hybrid XRD–XAS measurements, validating that the structural models reproduce key features of the real material before their electronic properties are examined. Within these models, the calculated electronic structure shows signatures of localized, hole-like small polarons trapped on oxygen ions. Additionally, rather than appearing as a generic feature of the pristine layered structure, these oxygen-centered states emerge only in specific local structural and conditions. In particular, partial delithiation of local regions is required to create the relevant charge imbalance while TM_LI anti-site defects provide a local environment that stabilizes polaron trapping on oxygen. The results highlight the importance of predicting not only the average crystal structure of NMC cathodes, but also the local defect configurations that determine their electronic response. Thus, by linking cation ordering, lithium-vacancy environments, anti-site formation and oxygen-centered polarons, this work contributes to structural prediction towards understanding the highly correlated relationship between structure and property in complex battery materials.

M25 - Magnetism Research in the Central Europe Region

M25 – Session 1 (Wed 23, 10:30-12:30, Chair: Neven Barišić)			
ID	Title	Speaker	Type
1591	**Magneto-optical detection of time-reversal symmetry breaking in antiferromagnets**	Veronika Sunko	Invited talk (10:30-11:00)

Veronika Sunko (1)

(1) Insitute of Science and Technology Austria (ISTA)

Optical probes are naturally well suited to detecting broken symmetries, including time-reversal symmetry (T), and are frequently used in this way, for example, to map ferromagnetic domains. But the conditions under which optics can detect T - breaking in antiferromagnets with no net magnetization are far more subtle. The key distinction is whether the effect of T can be undone by a simple translation (S_(1/2)); if it can, the product 〖TS〗(1/2) is a symmetry of the system and T-breaking is usually invisible to bulk probes. In contrast, antiferromagnets that do not preserve 〖TS〗(1/2) display a range of bulk T-breaking phenomena, such as the magnetoelectric and piezomagnetic effect.
But what exactly does "bulk" mean? And more specifically, are optical probes "bulk": can they detect T- breaking in 〖TS〗(1/2) - invariant antiferromagnets? We address these questions by comparing three antiferromagnets: non-collinear EuIn2As2 and altermagnetic MnTe that break 〖TS〗(1/2) and MnBi2Te4 that does not. In EuIn2As2 we show how an unconventional optical probe, linear magneto-birefringence, can reveal symmetry breaking invisible to more standard measurements [1-3]. In MnTe, simultaneous measurements of linear and circular dichroism reveal microscopic orientation of the T - breaking order parameter [4]. In MnBi2Te4, we demonstrate how perhaps the most standard optical probe of magnetism, reflection circular dichroism, can in fact detect antiferromagnetism even when 〖TS〗_(1/2) is preserved in the bulk [5].
Together, these experiments demonstrate both the power and the versatility of optics as a probe of symmetry breaking in quantum materials.

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[3] Sunko, V.; Orenstein, J., arXiv, 2511.16421 (2025)
[4] Liebman-Peláez, A.; Kruppe, J.; Regmi, R. B.; Ghimire, N. J.; Sun, Y.; Mazin, I. I.; Noad, H. M. L.; Analytis, J.; Sunko, V.; Orenstein, J., arXiv, 2604.07653, (2026)
[5] Sunko, V.; Ahsanullah, S.; Jain, V.; Weber, S.; Kumaran, S.; Yan, J.-Q.; Orenstein, J.; Ovchinnikov, D., arXiv, 2504.16167 (2025)

573	**Spin transport in antiferromagnets and altermagnets**	Helena Reichlova	Invited talk (11:00-11:30)

Helena Reichlova (1)

(1) FZU Czech Academy of Sciences

Ferromagnets have long been the foundation of spintronics applications. However, materials with compensated magnetic order, such as antiferromagnets, offer distinct advantages, including faster dynamics and a wider range of available materials. This has spurred significant research into antiferromagnetic spintronics, leading to many exciting discoveries [1]. Despite these advancements, antiferromagnets are often not considered robust sources of coherent spin currents. Recently, a new class of compensated magnets, altermagnets, has been identified, combining key advantages of both ferromagnets and antiferromagnets and offering promising potential for spintronics applications [2,3].
In this talk, I will briefly discuss the key experiments of antiferromagnetic spintronics and after that I will introduce the concept of altermagnetism and present several materials that can host altermagnetic order and that we have studied experimentally [4–6]. I will discuss our studies of electronic spin transport in these systems, including the observation of the anomalous Hall effect in a single layer of an altermagnetic material and its thermoelectric counterpart, the anomalous Nernst effect [7]. Next, I will focus on heterostructures containing altermagnets and show that they can behave similarly to ferromagnets in generating robust spin currents [7]. Finally, I will discuss the implications of altermagnetism for magnon-mediated spin currents [8].

[1] T. Jungwirth et al., Nature Nanotechnology 11, 231–241 (2016)
[2] L. Šmejkal et al., Physical Review X 12, 040501 (2022)
[3] C. Song, HR et al., Nature Reviews Materials, 1–13 (2025)
[4] R. D. Gonzalez Betancourt, HR et al., Physical Review Letters 130, 036702 (2023)
[5] H. Reichlová et al., Nature Communications 15, 4961 (2024)
[6] A. Badura, HR et al., Nature Communications 16, 7111 (2025)
[7] J. Mencos, HR et al., arXiv:2512.17427
[8] M. Leiviskä, HR et al., Physical Review Materials 9, 084403 (2025)

583	**Dynamics of proximity- induced magnetism at cobalt/molecular interfaces**	Tomaž Mertelj	Invited talk (11:30-12:00)

Tomaž Mertelj (1) Mattia Benini (2) O. Cespedes (3) M. Cinchetti (4) V. A. Dediu (2) Gregor Jecl (1) Viktor V. Kabanov (1) S. Ozdemir (3) U. Parlak (4) R. K. Rakshit (2) M. D. Rogers (3) Andrei V. Shumilin (1) Jaka Strohsack (1) Hui Zhao (1)

(1) Jozef Stefan Institute
(2) ISMN-CNR
(3) University of Leeds
(4) Technische Universität Dortmund

The hybridized layer at the interfaces between a magnetic metal and another material represents one of the important low dimensional paradigms offering a method for tailoring magnetic properties of ultrathin metallic layers. In the case of molecular semiconductors the hybridization between the molecular p orbitals and the d orbitals of the interfacial metallic atoms modifies both the molecules and the interfacial atomic layer of the metal. This manifests itself in significantly altered low-temperature magnetic properties of layered metal/molecules heterostructures [1–3].
Although the influence of organic molecules on the magnetic properties of thin metallic films has been investigated for decades [1,2,4,5], a precise understanding of the magnetism and hybridization at the interface is still lacking. We provide further insight into the physics of such interfaces through

systematic investigations of the magnetic dynamics in layered structures composed of molecular semiconductors and cobalt using ultrafast magneto-optical spectroscopy. Combined with the development of a theoretical model, we unveil [6] the existence of an independent magnetic component at the interface, which could not be extracted using the standard static methods. We also show that the properties of this component can be effectively modulated by short optical pulses [7] enabling control over the direction of magnetization in the cobalt layer [8].

[1] K. Bairagi et al., Phys. Rev. Lett. 114, 247203 (2015).
[2] T. Moorsom et al., Phys. Rev. B 90, 125311 (2014).
[3] M. Benini et al., Nat Commun 16, 5807 (2025).
[4] Z. H. Xiong et al., Nature 427, 821 (2004).
[5] S. Sanvito, Nature Phys 6, 562 (2010).
[6] J. Strohsack et al., Science Advances 11, eadw2243 (2025).
[7] M. Benini et al., Nat Commun 16, 7297 (2025).
[8] S. Ozdemir et al., Advanced Materials n/a, e19192.

542	**A theoretical study of vibrational magnetism: From molecular pseudorotation to dynamical multiferroicity in the bulk**	Matthias Diez	Contributed talk (12:00-12:15)

Matthias Diez (1) Johannes Krondorfer (1) Andreas Hauser (1)

(1) Graz University of Technology

The recent surge of interest in chiral phonons – vibrational modes carrying angular momentum – brings renewed attention to the interplay between magnetism and atomic or molecular motion. While current studies focus mostly on bulk materials, molecular systems provide an ideal, well-controlled platform for the exploration of similar phenomena on the microscopic scale. In this work, we present a comprehensive and rigorous theoretical study of vibrational magnetism in molecules, originating from the coupling between nuclear motion and magnetic moments.
Phenomena related to rotational and vibrational magnetism in molecules were already explored over half a century ago, particularly during the early development of microwave spectroscopy. However, a consistent and quantitative theoretical framework describing spin–vibration interactions has remained incomplete. By combining modern ab initio computational techniques with analytical modeling to extract the relevant coupling parameters, we revisit this longstanding problem and predict the emergence of localized magnetic fields induced by molecular vibrations.
While our current analysis focuses on interactions involving nuclear spins, the framework we develop can be naturally extended to include electron spins. This opens up new directions for understanding and exploring the rapidly developing field of chiral phononics.

191	**Theoretical framework for polarization dependent magneto-absorption in (anti)ferromagnetic materials**	Stáňa Tázlarů	Contributed talk (12:15-12:30)

Stáňa Tázlarů (1) Sigurður Erlingsson (2) Karel Výborný (3)

(1) Faculty of Mathematics and Physics, Charles University, Prague
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(3) Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, Praha 6, CZ-16253, Czech Republic

Microscopic structure of (anti)ferromagnets (A)FMs can be described using Heisenberg spin Hamiltonians, with corresponding parameters such as spin-spin exchange couplings or anisotropies. Experimental determination of these parameters typically involves measurement of magnetic excitation spectra either via inelastic neutron scattering(INS) or (THz)GHz magneto-absorption.
While the absorption experiments provide greater accuracy than INS, they are limited to the Γ-point (k = 0) only, making the inclusion of external magnetic field H vital to extend the available dataset. Another avenue, which remains largely unexplored in the present literature, is the polarization control of the applied (THz)GHz field.
We utilize both numerical spin dynamics model and analytical description of the linear response regime in the linear spin wave theory(LSWT) framework to determine the circularly polarization(CP) dependent absorption coefficient and derive expressions connecting microscopic parameters of simple FMs and AFMs to features of resulting measurable magneto-absorption curves.

M26 - 2D Material Research in the Central Europe Region

M26 – Session 1 (Wed 23, 16:00-18:00, Chair: Tomáš Bzdušek)			
ID	Title	Speaker	Type
572	**Graphite-gate-defined devices in bilayer graphene**	Andrea Hofmann	Invited talk (16:00-16:30)

Francesco Blanda (1) Aurin Strathmann (1) Fabrizio Volante (1) Kenji Watanabe (2) Takashi Taniguchi (2) Klaus Ensslin (3) Thomas Ihn (3) Andrea Hofmann (1)

(1) University of Basel
(2) NIMS Japan
(3) ETH Zürich

Working with 2D materials, major limitations are imposed by device reproducibility and yield. The complexity in the fabrication gives rise to an immense number of parameters that have to be controlled. In bilayer graphene devices, the mastery of this parameter space is, to some extent, reflected by the opening of a uniform band-gap under the application of an electric field perpendicular to the bilayer sheet. This gap is theoretically expected and routinely achieved in experiments, but its leanliness as measured by the in-gap resistance is of varying quality and strongly depends on the fabrication details. Clean gaps allow for separating the device from insulating regions by electrostatically gating the Fermi level into the bandgap instead of etching away the material. In the latter approach, the resulting device edges are highly disordered [1], and even though electrostatic device definition has allowed for measurements of clean quantum point contacts [2] and quantum dots [3,4], the device edges themselves have remained less explored. In addition, little attention has been paid to the natural flake edges, which may still provide some conducting paths in typical gate-defined geometries.
In our attempt to increase device yield and reproducibility, we have conceived a new design of dual-gated bilayer graphene devices. Taking into consideration concerns about Cr and Ti sticking layers [5] and following recent trends in the field [6,7], we move away from metal as top-gate electrode, but instead rely on graphite layers. Our devices are designed in a way that keeps the active area unaffected from exposure to polymers or high-voltage electron beams used in typical lithography processes. Importantly, the active area is fully isolated from the natural flake edges. We characterize our device architecture by performing magnetotransport measurements on different device geometries, including field-effect transistors, a Hall bar, and an Aharonov-Bohm ring. We assess the general device quality by extracting band-gap resistance and uniformity, mobility, and coherence length. In addition, we perform detailed analyses on the scattering effects at the device boundaries and discuss the parameter regimes in which nano-scale devices like quantum dots are preferably operated.

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[2] H. Overweg, H. Eggimann, X. Chen, S. Slizovskiy, M. Eich, R. Pisoni, Y. Lee, P. Rickhaus, K. Watanabe, T. Taniguchi, V. Fal'ko, T. Ihn, and K. Ensslin, Nano Lett. 18, 553 (2018).
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[4] L. Banszerus, B. Frohn, A. Epping, D. Neumaier, K. Watanabe, T. Taniguchi, and C. Stampfer, Nano Lett. 18, 4785 (2018).
[5] W. Zheng, K. Zhu, S. Pazos, Y. Shen, Y. Yuan, O. Alharbi, Y. Ping, and M. Lanza, Appl. Surf. Sci. Adv. 29, 100820 (2025)
[6] A. A. Zibrov, C. Kometter, H. Zhou, E. M. Spanton, T. Taniguchi, K. Watanabe, M. P. Zaletel, and A. F. Young, Nature 549, 360 (2017).
[7] E. Icking, D. Emmerich, K. Watanabe, T. Taniguchi, B. Beschoten, M. C. Lemme, J. Knoch, and C. Stampfer, Nano Lett. 24, 11454 (2024).

757	**Tuning van der Waals heterostructures with pressure**	Péter Makk	Invited talk (16:30-17:00)

Péter Makk (1)

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In van der Waals heterostructures the layer distance strongly affects the interaction between the layers. Therefore, pressure is an ideal tool to engineer the band structure of van der Waals materials [1].
Here I will show examples for the versatility of this method. First, I will show, how in WSe2/Gr structures spin-orbit coupling can be boosted using hydrostatic pressure [2-4]. I will also demonstrate the effect in 2D magnetic materials, where pressure allows the tunability of both the magnetic phase diagram, both the transport processes [5]. Finally, I will demonstrate the band structure tuning of magic-angle twisted bilayer graphene [6]. The pressure has a strong effect on the flat band structure and leads to changes both superconducting and in topological states.

[1] B. Fülöp et al., Journal of Applied Physics 130, 064303 (2021)
[2] B. Fülöp et al., npj 2D Materials and Applications 5, 82 (2021)
[3] M. Kedves et al., Nano Letters., 23, 9508 (2023)
[4] Bálint Szentpéteri, et al., Phys. Rev. B 111, 205415 (2025)
[5] Albin Marffy et al., Nano Letters, 26, 5, 1782–1788 (2026)
[6] B. Szentpéteri et al., Nano Letters, 21, 8777 (2021)

586	**Strong charge–photon coupling and simulation-guided design in low-dimensional quantum dot systems**	Marián Janík	Invited talk (17:00-17:30)

Marián Janík (1,2) Kevin Roux (1) Carla Borja Espinosa (1) Oliver Sagi (1) Abdulhamid Baghdadi (1) Thomas Adletzberger (1) Andrea Ballabio (3) Marc Botifoll (4) Alba Garzón Manjón (4) Jordi Arbiol (4,5) Daniel Chrastina (3) Giovanni Isella (3) Ioan Pop (6) Georgios Katsaros (1) Peter Stano (2,7)

(1) Institute of Science and Technology Austria
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(3) Politecnico di Milano
(4) Catalan Institute of Nanoscience and Nanotechnology
(5) Catalan Institution for Research and Advanced Studies
(6) Karlsruhe Institute of Technology
(7) RIKEN Center for Emergent Matter Science

Charges and spins confined in semiconductor quantum dots coupled to microwave photons provide a versatile platform for quantum computation and quantum optics, but coupling strengths are fundamentally limited by the weak electric dipole moment. In this context, heterostructures hosting low-dimensional carrier systems offer a promising route to scalable and tunable architectures.

Here, we investigate quantum dots defined in germanium quantum wells, where a high-mobility two-dimensional hole gas enables strong confinement and electrical control. By integrating these heterostructures with high-impedance granular aluminium superconducting resonators, we enhance the charge--photon interaction and achieve strong coupling.
The large kinetic inductance of granular aluminium allows us to realize resonators with characteristic impedances exceeding 20 k, significantly boosting the dipole coupling strength and overcoming a key limitation of semiconductor circuit quantum electrodynamics.
In parallel, we develop numerical electrostatic models of gate-defined quantum dots, enabling systematic optimization of device geometry via charge distributions, lever arms, and dipole moments. These simulations provide a predictive framework for engineering device performance.
The combination of materials engineering and simulation-guided design establishes a scalable approach to quantum device optimization, directly applicable to a broad class of low-dimensional material platforms.

630	**Investigation of rhombohedral multilayer graphene via tunable moiré superlattices**	Matheo Ablasser	Contributed talk (17:30-17:45)

Matheo Ablasser (1) Kenji Watanabe (2) Takashi Taniguchi (2) Hryhoriy Polshyn (3) Silke Paschen (1) Fangyuan Yang (1)

(1) Institute of Solid State Physics, TU Wien
(2) NIMS Japan
(3) Institute of Science and Technology Austria

Rhombohedral multilayer graphene (RMG) exhibits a rich phase diagram with a variety of magnetic, superconducting, and topological phases, making it a highly interesting material for current condensed matter research. In addition, the introduction of a moiré pattern can reveal further emergent phenomena. For example, RMG with an imposed moiré potential by an hBN substrate has been shown to host a fractional quantum anomalous Hall effect [1]. However, in this architecture the moiré pattern is fixed during fabrication and cannot be tuned afterwards, limiting systematic studies and exploration of correlated phases in RMG.
In this talk, we present the fabrication process and first characterization of a novel device designed to study the properties and phase diagram of RMG using a tunable moiré superlattice. This approach aims to systematically investigate the highly correlated electron system. This talk will discuss the device design, fabrication challenges, preliminary measurements, and the outlook for future experiments.

[1] Zhengguang Lu et al., “Fractional Quantum Anomalous Hall Effect in Multilayer Graphene,” Nature 626, 759-764 (2024).

361	**Broadband Charge Transport in 2D $Ti_3C_2T_x$ MXene Thin Films: From D.C. to 80 THz**	Kunal Tiwari	Contributed talk (17:45-18:00)

Kunal Tiwari (1) Rostislav Matuška Matuška (1) Hong Dang Nguyen Nguyen (1) Hynek Němec Němec (1) Petr Kužel Kužel (1)

(1) Institute of Physics of the Czech Academy of Sciences, Prague Czech Republic

Probing charge carrier dynamics across a broad frequency range — from terahertz (THz) to infrared (IR) regimes — presents a powerful, contact-free procedure to investigate nanoscale transport phenomena in low-dimensional materials. Combining frequency dependent optical conductivity spectra with conventional d.c. electrical measurements enable a comprehensive picture of carrier transport mechanisms in morphologically complex systems such as solution processed 2D materials.
Here, we report a systematic investigation of charge transport in thin films of 2D $Ti_3C_2T_x$ MXene over an exceptionally wide spectral range (d.c. + 0.3 - 80 THz). Films of varying thickness were fabricated by convection-assisted self-assembly at the liquid–air interface, yielding well-controlled 2D flake networks on semi-insulating Si substrates. Non-zero d.c. conductivity across all samples confirms a percolated network, validated by microstructure analysis via. optical and electron microscopy. Systematic increase of the real conductivity in the frequency range ~ 0.2 - 16 THz reveals partial carrier localization. Broadband fitting using the modified Drude-Smith model demonstrates a clear correlation between the localization rate and the characteristic MXene flake size. At higher frequencies, a crossover to intrinsic Drude behavior — marked by decreasing conductivity and increasing optical transparency — is observed. We further discuss the systematic evolution of transport parameters as a function of film thickness, providing design guidelines for MXene-based optoelectronic and electromagnetic applications.

M26 – Session 2 (Thu 24, 10:30-12:30, Chair: Wolfgang Lang)

ID	Title	Speaker	Type
771	**Chiral states in classical and quantum spin models**	Karlo Penc	Invited talk (10:30-11:00)

Karlo Penc (1) Judit Romhányi (2) Yasir Iqbal (3) Péter Kránitz (4)

(1) HUN-REN Wigner Research Centre for Physics
(2) UC Irvine, Irvine, USA
(3) Indian Institute of Technology Madras
(4) Budapest University of Technology and Economics

Frustrated magnets provide fertile ground for unconventional orders and emergent excitations. In particular, chiral states break time-reversal symmetry and host emergent gauge fluxes that can endow quasiparticles with nontrivial topology [1,2,3]. Here, we explore two complementary aspects: topological magnon transport and exactly solvable spin models.
On the triangular lattice, we study a spin-1/2 isotropic Heisenberg model with further-neighbor exchanges and ring exchange. The four-site ring exchange stabilizes a chiral four-sublattice noncoplanar order, which generates finite Berry curvature in the magnon bands and produces a thermal Hall effect even without Dzyaloshinskii-Moriya interactions. Using variational methods, we further show that this ordered phase can melt into a chiral spin liquid, continuously connected to the $U(1)$ Dirac spin liquid in the absence of ring exchange.
On corner-sharing tetrahedral lattices, we construct local frustration-free parent Hamiltonians whose exact ground-state manifolds contain chiral four-coloring spin configurations. These states generalize ice-rule constraints to a finite set of noncoplanar spin directions and possess intrinsic scalar chirality. For arbitrary spin-S, including the classical limit, the local Hamiltonian can be written as a positive-semidefinite form. Using a Schwinger-boson formulation,

we identify the structure of the zero-energy manifold and show that it contains an extensive degeneracy on checkerboard and pyrochlore lattices. Our construction provides a systematic route to stabilizing chiral phases in frustrated quantum magnets.

571	**Interface-engineered switchable polar states down to a single unit cell**	Nives Strkalj	Invited talk (11:00-11:30)

Nives Strkalj (1)

(1) Institute of Physics, Zagreb

Controlling ferroic order at the nanoscale is central to the development of next-generation low-power electronic and spintronic devices. I will present our recent work on interface-engineered phenomena in complex oxide heterostructures based on $BaTiO_3$ and $La_{0.67}Sr_{0.33}MnO_3$. Through interface charge design, we realize switchable polar states down to a single unit cell of $BaTiO_3$ in superlattice and trilayer architectures. These results show that interface charge engineering can overcome critical thickness limits in ultrathin perovskite films. We thereby provide a pathway toward harnessing their low coercive fields for energy-efficient electronics.

525	**Excitonic Effects Modeling in van der Waals Heterostructures of 2D Materials**	Frantisek Karlicky	Invited talk (11:30-12:00)

Frantisek Karlicky (1)

(1) University of Ostrava

We review here our achievements in the field of excitons in van der Waals (vdW) heterostructures of two-dimensional (2D) materials from the last few years. Electron-electron and electron-hole (exciton) effects are specifically pronounced in 2D materials and their vdW heterostructures due to weak dielectric screening from the environment. These heterostructures offer a versatile platform for engineering excitonic and optoelectronic properties. However, accurate prediction of their behavior is non-trivial. We show that a) advanced many-body methods are indispensable for these systems [1]; b) reliance on standard commensurate models introduces artificial strain, creating a significant risk of misattributing computational artifacts to intrinsic interface physics [2]; and c) in certain vdW heterostructures, the emergence and energy of interlayer excitons depend sensitively and predictably on the stacking order [3]. From a computational point of view, our work uses very accurate many-body methods (GW, BSE, TD-DFT) to resolve subtle physical effects between and within layers. We proved these techniques to be precise at the experimental level or compatible with independent stochastic approaches (QMC), also for 2D materials [4-7]. Our findings highlight how stacking-dependent interlayer coupling governs key excitonic properties of vdW heterostructures, allowing targeted manipulation for tailored next-generation light-harvesting and quantum technologies.

[1] Ketolainen T., Macháčová N., Karlický F.: Optical Gaps and Excitonic Properties of 2D Materials by Hybrid TD-DFT: Evidences for Monolayers and Prospects for vdW Heterostructures. J. Chem. Theory Comput. 16 (2020) 5876
[2] Macháčová N., Kalmár J., Karlický F.: Excitonic landscape and quasi-type-I nature of incommensurate Ti-based MXene/MoS van der Waals heterostructures. Under review (2026)
[3] Kumar N., Kolos M., Karlický F.: Stacking-Dependent Interlayer Excitons in BP/CrSe van der Waals Heterostructure. Nano Lett. 25 (2025) 16608
[4] Kolos M., Karlický F.: Predicting Fundamental Gaps of Chromium-Based 2D Materials Using GW Methods. J. Phys. Chem. C 129 (2025) 2782
[5] Kumar N., Karlický F.: Oxygen-terminated TiC MXene as an excitonic insulator. Appl. Phys. Lett. 122 (2023) 183102
[6] Dubecký M., Karlický F., Minárik S., Mitas L.: Fundamental gap of fluorographene by many-body GW and fixed-node diffusion Monte Carlo methods. J. Chem. Phys. 153 (2020) 184706
[7] Dubecký M., Minárik S., Karlický F.: Benchmarking fundamental gap of ScC(OH) MXene by many-body methods. J. Chem. Phys. 158 (2023) 054703

Acknowledgements: This contribution has been produced with the financial support of the European Union under the LERCO project (number CZ.10.03.01/00/22_003/0000003) via the Operational Programme Just Transition.

635	**Quantum sensing of a nanoscale electronic phase segregation in an oxygen-deficient Mn-doped $CaFe_3O_5$ perovskite oxide**	Izidor Benedičič	Contributed talk (12:00-12:15)

Denis Arčon (1) J. Paul Attfield (2) Izidor Benedičič (1) Ka H. Hong (2)

(1) Jožef Stefan Institute
(2) University of Edinburgh

Doping of transition metal oxides provides a controlled route for tuning the charge, spin, and lattice degrees of freedom, thereby enabling the tailoring of magnetic and electronic functionalities of the material. However, local probe studies of powder samples remain challenging due to strong electron correlation effects and charge/spin dynamics, obscuring the fine spectroscopic properties. Weakly doped high-pressure-grown $CaFe_3O_5$ was shown to segregate into two distinct electronic phases with different antiferromagnetic orderings. At the same time, the samples exhibit weak ferromagnetism, likely arising from canting of spin chains, and the relationship between ferromagnetism and phase segregation remains an open question.
For the study of Mn-doped $CaFe_3O_5$, we employ quantum magnetometry based on nitrogen-vacancy (NV) centres in nanodiamonds, impressed into the doped $CaFe_3O_5$ powder pellet to probe both static and dynamic magnetic fields across the weak ferromagnetic transition. The optically detected magnetic resonance (ODMR) spectra of the NV ensemble show additional broadening and splitting below the critical transition temperature T_c = 290 K. At the same time, the spin-lattice relaxation increases drastically at T_c, a signature of enhanced magnetic fluctuations.
Microscopic modelling of ODMR spectra reveals signatures of a weakly ferromagnetic phase coexisting with an antiferromagnetic phase. By relating the magnetic spectra with electronic phase fractions determined from neutron scattering, we find the majority phase to be a likely candidate for spin canting, resulting in weak ferromagnetism. The presented study demonstrates the viability of using nanodiamonds as a low-cost platform for magnetic measurements in solid-state systems.

536	**Stress induced uniaxial magnetic anisotropy in AlScN/CoFeB magnetoelectric thin films**	Manoj Matpathi	Contributed talk (12:15-12:30)

Manoj Matpathi (1) Luiz Enger (1) Amalio Fernandez-Pacheco (2) Takeaki Gokita (2) Sabri Koraltan (3) Sanjay Nayak (1) Balram Singh (2) Le Zhao (2)

(1) Silicon Austria Labs, Villach, Austria
(2) Physics of 3D nanomaterials, IAP, TU-Wien, Vienna, Austria

(3) Institute of Applied Physics, Technische Universität Wien

The magnetoelectric (ME) effect utilizes strain-mediated coupling between magnetostrictive and piezoelectric layers for electric-field control of magnetization and magnetic-field control of strain. Recently, ME effect has gained attention due to its wide range of applications in magnetic field sensors, spintronic and RF devices. Hence, it is vital to understand how various parameters influence the coupling between piezoelectric and magnetostrictive layers for the improvement of ME devices.
In this work, the influence of the residual stress induced during depostion of AlScN(500nm) layer on a 10 nm thick CoFeB magnetostrictive layer was investigated. AlScN was selected as the piezoelectric material due to its compatibility with the standard CMOS processes. Although CoFeB has been extensively studied in conjunction with other piezoelectric substrates 1, its behaviour when interfaced with AlScN remains unclear.
To characterize the presence of in-plane magnetic anisotropy in the CoFeB layer grown on top of AlScN, hysteresis loops were measured using a vibrating sample magnetometer (VSM) by varying azimuthal in-plane angle (ϕ). The polar plot of coercivity (Hc) vs ϕ confirmed the presence of stress induced uniaxial anisotropy (along $\phi = 60°$) in case of AlScN/CoFeB/Ta ME stack. Atomic force microscopy (AFM) revealed the presence of abnormally oriented grains (AOGs) in the AlScN layer. The increased coercive field near the hard axis (along $\phi = 150°$) is attributed to the misalignment of local grain anisotropy 2. The influence of different seed layers such as Ta and Pt was also studied. The results presented here are the first steps for further development of high-quality magnetoelectric composites and the future direct integration of ME devices with CMOS technology.

This work has received funding from the European Union under the MSCA COFUND project CRYSTALLINE, grant agreement no. 101126571.

1 Millo, Florian, et al. "Symmetry of the dissipation of surface acoustic waves by ferromagnetic resonance." AIP Advances 15.4 (2025).
2 Idigoras, O., et al. "Collapse of hard-axis behavior in uniaxial Co films." Physical Review B—Condensed Matter and Materials Physics 84.13 (2011): 132403.

M27 - 2D Materials-Synthesis, Surfaces, Dynamics, Devices

M27 – Session 1 (Wed 23, 10:30-12:30, Chair: Anna Galler)			
ID	Title	Speaker	Type
230	**From Strong to Weak Correlations in Breathing-Mode Kagome van der Waals Materials—$Nb_3(F,Cl,Br,I)_8$ as a Robust and Versatile Platform for Many-Body Engineering**	Malte Rösner	Invited talk (10:30-11:00)

Malte Rösner (1)

(1) Bielefeld University

Understanding how electron correlations intertwine with topological properties of a crystal structure is a central challenge in quantum materials research. In this talk, I will discuss the family of breathing kagome compounds Nb3X8 (X = F, Cl, Br, I) as a versatile platform for exploring this interplay. Building on our recent work, I will first show how monolayer Nb3Cl8 constitutes an almost ideal realization of a single-orbital Mott–Hubbard insulator when described in a molecular orbital basis, with its low-energy physics fully captured by a one-band Hubbard model. I will then extend this perspective to the broader Nb3X8 series, where ab initio downfolding combined with cluster dynamical mean-field theory reveals a systematic evolution from weakly to strongly correlated states across the halogen series. The low-temperature bulk phases display tunable Coulomb- and Mott-driven gaps, suppressed electron–phonon coupling, and interlayer dimerization effects that yield magnetically singlet-like ground states. Finally, I will outline how these correlation-driven symmetry-breaking phenomena in Nb3X8 can influence quantum transport, providing new insights into the recently observed field-free Josephson diode effect in NbSe2/Nb3X8/NbSe2 heterojunctions. This connection highlights how correlated kagome systems can serve as a versatile platform for emergent functionalities in many-body driven devices.

143	**A first-principles framework for strain-driven exciton transport in 2D TMDs**	Amir Kleiner	Contributed talk (11:00-11:15)

Amir Kleiner (1) Sivan Refaely-Abramson (1)

(1) Weizmann Institute of Science

In many two-dimensional semiconductors, spatially varying strain profiles provide a powerful means to induce and steer exciton motion, yet a predictive microscopic description of the resulting dynamics remains limited. Here, we present a general first-principles framework for exciton dynamics in inhomogeneous materials. Our approach combines GW-BSE calculations of strain-dependent excitonic band structures with a continuous position- and momentum-dependent potential landscape, thereby coupling real-space and reciprocal-space dynamics within a unified description.
We demonstrate the framework for the representative case of two-dimensional materials, focusing on the illustrative limit of propagation in the absence of scattering. More broadly, however, the method is not restricted to 2D systems and can be naturally extended to materials of any dimensionality, as well as to additional interaction channels and scattering mechanisms whenever the relevant quantities are available on compatible momentum- or real-space grids. Applying the approach to representative strain profiles in 2D transition-metal dichalcogenide monolayers, we qualitatively reproduce experimentally observed phenomena such as directed exciton drift toward regions of higher strain, as well as nontrivial transport and broadening behavior that provide a microscopic interpretation of previously reported anomalous drift and diffusion. These results show how band-structure renormalization and local strain gradients jointly govern exciton transport, and establish a versatile route for predicting and engineering quasiparticle dynamics in 2D materials and beyond.

402	**Solving the Phase Problem of Diffraction: XSW Imaging on Bismuthene/SiC(0001)**	Serguei Soubatch	Contributed talk (11:15-11:30)

Fabian Göhler (1) Christian Kumpf (2) Tien-Lin Lee (3) Philip Schädlich (1) Thomas Seyller (1) Sergey Subach (2) Frank Stefan Tautz (2,4) Niclas Tilger (1) Susanne Wolff (2)

(1) Institute of Physics, Chemnitz University of Technology
(2) Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich
(3) Diamond Light Source, United Kingdom
(4) RWTH Aachen, Germany

For the quantum spin Hall insulator bismuthene, robust helical edge states protected by a large topological band gap of 800 meV have been demonstrated, making the system interesting for potential room-temperature spintronic applications [1]. Here, we show that a single layer of elemental Bi, formed by intercalating an epitaxial graphene buffer layer on SiC(0001), can be transformed into bismuthene [2]. Specifically, the layer of atomic Bi can be reversibly switched between an electronically inactive precursor state and a state that exhibits the predicted band structure of a true two-dimensional bismuthene. This switching is accomplished by enabling/disabling a partial hydrogen-passivation of Si dangling bonds, which triggers a change of the Bi adsorption site. This key finding describing the mechanisms behind bismuthene formation and switching, was achieved using normal incidence x-ray standing wave imaging (NIXSWI) [2]. Diffraction-based techniques, which are conventionally used to resolve atomic structure, are limited by the so-called "phase problem". Specifically, they are capable of determining the diffraction intensities, which represent the squared magnitudes of the complex structure factors. On the contrary, NIXSWI is a “direct method” for structure determination because it measures both the amplitudes and phases of the structure factors. It overcomes the phase problem by exploiting the direct relationship between the phase of the structure factor and the phase of an x-ray standing wave field generated by the interference of the incoming wave and the selected Bragg wave reflected from a crystalline substrate. Although this method was proposed already 40 years ago [3], it was raraely applied due to its demanding experimental requirements. In our study, NIXSWI provides chemically specific atomic densities, directly resolving the structural configuration of bismuth before and after transformation.

[1] L. Gehrig et al., Adv. Mater. 37, 2502412 (2025)
[2] N. Tilgner et al., 2D Mat. 12, 045020 (2025), and Nat. Commun. 16, 6171 (2025)
[3] M.J. Bedzyk, G. Materlik, Phys. Rev. B 32, 6456 (1985).

760	**High-harmonic spectroscopy of a sliding ferroelectric**	Elias Greil	Contributed talk (11:30-11:45)

Anna Galler (1) Elias Greil (1) Alba de las Heras (2)

(1) TU Graz
(2) Max Planck Institute for the Structure and Dynamics of Matter (MPSD)

High-harmonic generation is a sensitive all-optical probe of symmetry and electron dynamics in solids. Here, we use first-principles time-dependent density functional theory (TDDFT) to study high-harmonic generation in T_d-WTe_2, a two-dimensional semimetal with switchable out-of-plane ferroelectric polarization driven by interlayer sliding. We show that the mirror-symmetry breaking underlying the ferroelectric state produces robust signatures in polarization-resolved high-harmonic spectra, enabling optical identification of the polarization state. By incorporating interlayer shear motion in coupled electron-lattice TDDFT simulations, we further show that the 0.24 THz shear mode is slow enough to remain effectively decoupled from the ultrafast electronic response responsible for harmonic emission. Our results establish high-harmonic spectroscopy as a non-invasive probe of sliding ferroelectricity and lattice symmetry in two-dimensional quantum materials.

227	**Benchmarking Edge Contacts for Sub-15 nm MoS_2 Transistors: Metal, Phase-Engineered, and Semimetal Approaches**	Mate Capin	Contributed talk (11:45-12:00)

Mate Capin (1) Lado Filipovic (1)

(1) Institute of Microelectronics, TU Wien, Vienna, Austria

As silicon CMOS technology approaches scaling limits, two-dimensional (2D) semiconductors such as molybdenum disulfide (MoS_2) are being explored for next-generation transistor channels due to their excellent electrostatic control and reduced short-channel effects. However, achieving low contact resistance remains a key challenge, as Fermi level pinning (FLP) and van der Waals gaps in conventional top-contact geometries lead to significant Schottky barriers.
In this work, we present a computational study based on density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) formalism to investigate edge-contact injection in MoS_2 transistors with channel lengths in the 12 – 15 nm regime. Three contact paradigms are benchmarked: conventional Au edge contacts, phase-engineered $1T' - 2H$ MoS_2 homojunctions, and semimetallic Bi contacts.
Using QuantumATK, we analyze the interfacial electronic structure and transport properties, focusing on band alignment, Schottky barrier formation, and interfacial transmission. Particular attention is given to the role of contact-induced states and orbital hybridization in facilitating carrier injection. The different contact paradigms are compared in terms of transmission efficiency and their ability to approach ohmic behavior in the short-channel regime.
By correlating atomistic interface properties with transport characteristics, this study identifies key interface features that mitigate Fermi level pinning and enhance carrier injection, providing insight into contact design strategies for sub-15 nm 2D electronic devices.

769	**Investigation of the vibrational, chemical and electrical properties of 2D-$GeCH_3$**	Zahra Kamranipour	Contributed talk (12:00-12:15)

Zahra Kamranipour (1) Saeed Rasouli (1) Behzad Dadashnia (1) Annette Foelske (2) Francesco Laudani (2) Daniele Nazzari (1) Matthew G. Panthani (3) Walter M. Weber (1)

(1) Institute of Solid-State Electronics, TU Wien, Vienna, 1040 Austria
(2) Service Unit of Analytical Instrumentation Center, TU Wien, Vienna, 1060 Austria
(3) Department of Chemical and Biological Engineering, Iowa State University, Ames, IA, USA

Germanane is a group IV, two-dimensional semiconductor, analogous to graphane, which is predicted to possess a direct bandgap. Its structure and properties can be tuned by surface functionalization, which can also increase the material's stability. Chemically synthesized crystals of methyl-terminated ($GeCH_3$) germanane are exfoliated via the scotch-tape method, and the resulting multilayered flakes are systematically investigated, focusing on their structural, chemical, thermal, and electrical characteristics. Raman spectroscopy and photoluminescence (PL) measurements reveal distinct vibrational modes characteristic of a germanium-based 2D material and emission features that confirm the presence of a direct band gap of approximately 1.75 eV. XPS analysis shows the expected Ge signature, without indication of Germanium oxidation. Furthermore, the thermal stability of $GeCH_3$ was examined through annealing studies in N2 and forming gas atmospheres, demonstrating a stability up to 200 °C. To explore the electronic performance, back-gated metal–oxide–semiconductor field-effect transistor (MOSFET) devices were fabricated. Initial electrical characterization shows clear light-dependent conductivity. These findings indicate that methyl-terminated germanane is a promising candidate for the realization of 2D-optoelectronics devices.

286	**Realizing Scalable Chemical Vapour Deposition of Monolayer Graphene Films on Iron with Concurrent Surface Hardening by in situ Observations**	Bernhard Bayer	Contributed talk (12:15-12:30)

Bernhard Fickl (1) Werner Artner (1) Daniel Matulka (1) Jakob Rath (1) Martin Nastran (1) Markus Hofer (1) Raoul Blume (2) Michael Hävecker (2) Alexander Kirnbauer (1) Florian Fahrnberger (1) Herbert Hutter (1) Dengsong Zhang (3) Paul Mayrhofer (1) Axel Knop-Gericke (2) Beatriz Roldan Cuenya (2) Robert Schlögl (2) Christian Dipolt (4) Dominik Eder (1) Bernhard Bayer (1)

(1) TU Wien
(2) FHI Berlin
(3) Shanghai University
(4) Rübig Gesellschaft m.b.H. & Co. KG

Graphene has been suggested as an ultimately thin functional coating for metallurgical alloys such as steels. However, even on pure iron (Fe), the parent phase of steels, growth of high quality graphene films remains largely elusive to date. We here report scalable chemical vapour deposition (CVD) of high quality monolayer graphene films on Fe substrates.[1] To achieve this, we here elucidate the mechanisms of graphene growth on Fe using complementary in situ X-ray diffractometry (XRD) and in situ near ambient pressure X-ray photoelectron spectroscopy (NAP XPS) during our scalable CVD conditions. As key factors that set Fe apart from other common graphene CVD catalyst supports such as Ni or Cu, we identify that for Fe (i) carbothermal reduction of persistent Fe-oxides and (ii) kinetic balancing of carbon uptake into the Fe during CVD near the Fe-C eutectoid because of the complex multi-phased Fe-C

phase diagram are critical. Additionally, we establish that the carbon uptake into the Fe during graphene CVD is not only important in terms of growth mechanism but can also be advantageously utilised for concurrent surface hardening of the Fe during the graphene CVD process, akin to carburization/case hardening. Our work thereby forms a framework for controlled and scalable high-quality monolayer graphene film CVD on Fe incl. the introduction of concurrent surface hardening during graphene CVD. Additionally, we will briefly introduce how such CVD graphene coatings can, depending on substrate, show a hithertho unreported controllable freezing transparency for water ice on scalable graphene films on metals.[2]

[1] B. Fickl, W. Artner, D. Matulka, J. Rath, M. Nastran, M. Hofer, R. Blume, M. Hävecker, A. Kirnbauer, F. Fahrnberger, H. Hutter, D. Zhang, P. H. Mayrhofer, A. Knop-Gericke, B. Roldan Cuenya, R. Schlögl, C. Dipolt, D. Eder, B. C. Bayer. Realizing Scalable Chemical Vapor Deposition of Monolayer Graphene Films on Iron with Concurrent Surface Hardening by In Situ Observations, ACS Appl. Mater. Interfaces, 18, 8567, (2026), https://doi.org/10.1021/acsami.5c18706
[2] B. Fickl, T. M. Seifried, E. Rait, J. Genser, T. Wicht, J. Kotakoski, G. Rupprechter, A. Lugstein, D. Zhang, C. Dipolt, H. Grothe, D. Eder, B. C. Bayer. Controllable Freezing Transparency for Water Ice on Scalable Graphene Films on Copper, arXiv, https://doi.org/10.48550/arXiv.2403.15629

M27 – Session 2 (Wed 23, 16:00-18:00, Chair: Anton Tamtögl)

ID	Title	Speaker	Type
753	**Tailoring the Interlayer Environment of Ti_3C_2 MXene for Sulfur Cathodes**	Asia Sarycheva	Invited talk (16:00-16:30)

Asia Sarycheva (1) Volker Presser (1,2,3)

(1) INM – Leibniz-Institut für Neue Materialien GmbH
(2) Department of Materials Science and Engineering, Saarland University, Saarbrücken, Germany
(3) saarene, Saarland Center for Energy Materials and Sustainability, Saarbrücken, Germany

Transition metal carbides and carbonitrides, MXenes, represent a unique class of 2D materials, where metallic electronic conductivity and redox-active surface coexist in a single material. This allows MXenes to function as "all-in-one" platforms for energy storage electrodes: the surface groups inherited from synthesis provide active redox centers. At the same time, the inherent electronic conductivity ensures efficient current flow throughout the electrode. The variety of atoms that can form MXenes, the control over flake stacking, and the ability to intercalate guest species provide three distinct degrees of freedom to tune this material family for specific applications.
Here, we showcase how engineering of the interlayer environment can be used through intercalation of a vast range of species, from Li^+ to CTAB. Because these processes occur in aqueous media, the solvation shell (rather than the bare ion) dictates the intercalation process. Consequently, the entrapment of structural water molecules together with the intercalant defines the local environment and the resulting material properties. We employ Raman spectroscopy to probe these interlayer interactions between Ti_3C_2 MXene and confined species.
To demonstrate how engineering of interlayer space affects material properties, we used the example of Li-S batteries. This chemistry is an attractive application as it allows for the use of a Li-metal anode—theoretically the electrode with the highest specific capacity (3860 mAh/g). In this system, the inherent challenges of the sulfur cathode require a conductive and structural host—a great task for MXenes. By varying the interlayer spacing and the affinity of intercalants to sulfur, we obtained various sulfur loadings and sulfur allotropic modification. By applying this material for cathodes in Li-S batteries, we demonstrate the power of interlayer engineering in 2D materials.

ID	Title	Speaker	Type
362	**Novel Mo_2C thin film synthesis approach towards electrochemical sensing applications**	Markus Eiberger	Contributed talk (16:30-16:45)

Markus Eiberger (1) Johannes Jeryczynski (1) Bernhard Fickl (1) Stefan Hummel (2) Christoph Wagner (2) Bernhard C. Bayer (1)

(1) Institute of Materials Chemistry, TU Wien, Vienna, Austria
(2) Badger Meter Austria GmbH, Vienna, Austria

Molybdenum Carbide (Mo2C) has a variety of useful properties and thus a lot of possible applications. Mo2C has good catalytic properties similar to the platinum metal group i.e. H2 production, water gas shift reaction or ammonia synthesis. In literature different approaches are reported to deposit thin films of Mo2C on substrates. Most commonly used are CVD systems with H2/Ar/CH4 flow and MoCl6, MoF6 or ammonium heptamolybdate tetrahydrate as precursor which require complex instrumentation and strict safety precautions. Further thin film methods use PVD and electrodeposition. Another CVD method obtains larger two-dimensional (2D) Mo2C crystals using molybdenum and copper metal-foils, Mo2C growing on liquid copper in H2/Ar/CH4 flow. This method is more limited because it can not be applied on substrates and difficulties of Mo2C transfer. We here present a new adaptation to such approach, simplifying the instrumentation and moving towards transfer-less uniform Mo2C coverage on functional substrates. The resulting Mo2C films may then be used in many applications, incl., e.g., electrochemical sensing applications.

ID	Title	Speaker	Type
382	**Polymer–2D Material Composite Coatings for Durable Solid Lubrication**	Martin Nastran	Contributed talk (16:45-17:00)

Martin Nastran (1) Maria Isabel Pérez (1) Hakan Göcerler (1) Bernhard Bayer (1) Pierluigi Bilotto (1) Carsten Gachot (1)

(1) TU Wien

Efficient lubrication is essential to reduce energy losses, minimise wear, and extend the lifetime of mechanical components. Solid lubricants, particularly layered two-dimensional (2D) materials, have attracted significant attention due to their low shear strength and unique interfacial properties. However, practical implementation remains challenging, as particulate lubricants exhibit poor adhesion to substrates and are rapidly removed from the contact interface during operation.
Among 2D materials, MXenes such as $Ti_3C_2T_x$ offer promising tribological performance but suffer from environmental instability, particularly hydrolysis under ambient conditions.[1,2] To address both adhesion and stability limitations, we systematically developed composite lubricating coatings by combining 2D materials with organic polymer matrices.
Layered materials, $Ti_3C_2T_x$, MoS_2, and graphite, were dispersed with fluorine-free polymers such as PMMA, PLA, PS, PIP, and PVDF via ultrasonic solution blending to form inks. These inks were deposited onto substrates using airbrushing and electrospraying techniques, yielding uniform coatings with significantly improved adhesion compared to pure powder films. Tribological testing reveals that polymer incorporation enables persistent lubrication by preventing lubricant loss from the interface. Soft polymer matrices provide moderate but stable friction reduction over extended sliding durations, whereas

harder polymers exhibit initially low friction coefficients but undergo rapid removal, limiting long-term performance. Notably, certain polymer systems partially suppress MXene degradation, enhancing environmental stability.
Despite these advantages, the exceptional lubricating properties of MXenes in powder form are not fully retained in the composite coatings, which underperform relative to polymer-free references.[3] This highlights the critical role of interfacial structure and matrix interactions in governing tribological behaviour. These findings demonstrate that while polymer-2D material composites offer a viable pathway toward durable solid lubrication, optimising matrix-filler interactions remains essential to fully exploit the potential of advanced 2D materials in tribological applications.

[1] Huang, S. & Mochalin, V. N. Hydrolysis of 2D Transition-Metal Carbides (MXenes) in Colloidal Solutions. Inorganic Chemistry 58, 1958–1966 (2019)
[2] Göçerler, H. et al. Unlocking the synergistic impact of laser texturing and Ti3C2Tx MXene coatings – Substrate-specific tribological insights. Carbon 238, 120270 (2025).
[3] Rosenkranz, A., Righi, M. C., Sumant, A. V., Anasori, B. & Mochalin, V. N. Perspectives of 2D MXene Tribology. Advanced Materials 35, 2207757 (2023)

693	**Enhancing the unusually strong electron-phonon kinks in hBN**	Justin Wells	Invited talk (17:00-17:30)

Justin Wells (1)

(1) University of Oslo

Background: In 2013, we reported strong electron-phonon coupling (EPC) in the σ-bands of graphene [1]. This observation was highly controversial at the time, and attempts were made to dismiss it as a consequence of photoemission matrix elements instead [2]. We endeavoured to clear up this controversy by i) theoretical support and ii) manipulating the photoemission matrix elements by measuring in the neighbouring BZs and on bilayer samples, confirming mass enhancements of $\lambda \approx 0.7$ [3].
Since then, we have predicted that hBN should host similarly strong EPC in its σ-bands [4]. This is unsurprising since the electronic structure, phonon structure, geometry, are all similar to graphene. On the other hand, experimental confirmation adds further credence to our understanding of EPC in graphene's σ-bands. Contrastingly, we predict strong EPC in the π-band of hBN. hBN's π-band has a parabolic maxima, making the EPC arguments (especially the scattering k-space) very different to graphene, and leading to much stronger EPC.
Most recently, we have confirmed the presence of strong EPC in both the π- and σ-bands of hBN. Furthermore, we show that the EPC strength in the π-band depends strongly on doping and/or substrate interaction, thus making it possible to further enhance the EPC (specifically with K and Cl intercalants). Several questions remain unanswered, and are the focus of ongoing work: including further ARPES studies, DFT and helium scattering studies.
In this talk, I will give a short overview of the unusual EPC in graphene's σ-bands, as well as presenting our most recent studies of monolayer hBN with dopants and intercalants. I will briefly present the helium scatting work and conclude with our latest understanding and some as yet unanswered questions.

[1] F Mazzola, et al., "Kinks in the Band of Graphene Induced by Electron-Phonon Coupling" Phys. Rev. Lett 111:216806 (2013)
[2] SW Jung et al., "Sublattice Interference as the Origin of σ Band Kinks in Graphene" Phys. Rev. Lett. 116:186802 (2016)
[3] F. Mazzola et al., "Strong electron-phonon coupling in the σ band of graphene" Phys. Rev. B 95:075430 (2017)
[4] E. Thingstad et al., "Phonon-mediated superconductivity in doped monolayer materials" Phys. Rev. B 101, p. 214513 (2020)

262	**Charge Transport and Neuromorphic Photoconductivity in 2D Single-Crystal Lead-Free PEA_2SnI_4**	Ofelia Durante	Contributed talk (17:30-17:45)

Ofelia Durante (1) Valeria Demontis (2) De Stefano Sebastiano (1) Daniela Marongiu (2) Adolfo Mazzotti (1) Selene Matta (2) Michele Saba (2) Giovanni Bongiovanni (2) Saverio Russo (3) Antonio Di Bartolomeo (1)

(1) Department of Physics 'E.R. Caianiello', University of Salerno, Via Giovanni Paolo II 132, Fisciano (SA) 84084,Italy
(2) Department of Physics – University of Cagliari, Monserrato (CA) 09042, Italy
(3) Centre for Graphene Science, College of Engineering, Mathematics and Physical Sciences – University of Exeter, Exeter, EX4 4QL UK

Lead-free 2D halide perovskites are promising materials for sustainable optoelectronics and neuromorphic photonics, but their intrinsic transport properties are often obscured in polycrystalline films by grain boundaries and Sn oxidation. Here, we investigate single crystals of PEA_2SnI_4 to clarify the interplay between surface degradation, charge transport, and photoresponse, extending previous studies on related 2D single-crystal perovskites such as PEA_2PbI_4 [1]. We find that air and light exposure mainly affect the surface, with partial recovery enabled by exfoliation. PEA_2SnI_4 devices exhibit strong visible-light photoconductivity, with responsivity up to 60 A W^{-1} under low-intensity 650 nm illumination. The sublinear power dependence indicates trap-assisted photoconductivity, while temperature-dependent measurements reveal a crossover around 225 K from thermally activated transport to phonon-scattering- and ion-migration-influenced conduction. Time-resolved photocurrent measurements further show persistent and cumulative responses typical of short-term synaptic plasticity. These results establish layered single-crystal perovskites as a versatile platform for investigating transport, degradation, and adaptive photoresponse in advanced optoelectronic systems [2].

[1] Demontis, V., Durante, O., et al. Advanced Optical Materials 13.6 (2025): 2402469.
[2] Durante, O., et al. Advanced Functional Materials (2025): e26339.

297	**Controlled growth of ultrathin 2D Mo_2C at lowered pressures**	Johannes Jeryczynski	Contributed talk (17:45-18:00)

Johannes Jeryczynski (1) Bernhard Fickl (1) Michael Hahn (1) Herbert Hutter (1) Gerlinde Habler (2) Bernhard Bayer (1)

(1) TU Wien
(2) Universität Wien

Since first being reported, the growth of two-dimensional (2D) metal carbides such as Mo2C via chemical vapour deposition (CVD) has received continuous attention from the research community. However, due to the complicated growth process involving a liquid metal catalyst, as well as process conditions also suitable for the concurrent growth of graphene, a multitude of different morphologies, heterostructures and respective growth mechanisms have been reported. So far, the system has almost exclusively been studied under ambient pressure growth conditions, making most common in-situ techniques such as in-situ near ambient pressure X-ray photoelectron spectroscopy (XPS) and environmental scanning electron microscopy (ESEM) inaccessible. In this work, we present recent advances in the development of low-pressure CVD growth of ultrathin Mo2C, studying various parameters of the system to tune grown crystals towards desired morphological properties.

M27 – Session 3 (Thu 24, 10:30-12:30, Chair: Bernhard Bayer)			
ID	Title	Speaker	Type
568	**Synthesis and Characterization of Two-Dimensional Diboron Trioxide Crystal Composed by Boroxol Groups**	Alessandro Sala	Invited talk (10:30-11:00)

Alessandro Sala (1)

(1) CNR - Istituto Officina dei Materiali (IOM)

Diboron trioxide (B_2O_3) represents a peculiar case among polymorphic oxides, for its vitrified state presents superstructural units – planar ring-shaped boroxol groups, B_3O_6 – that are totally absent in its crystalline polymorphs. In fact, the crystallization of B_2O_3 can occur only under applied pressure, where the boroxol groups can be disrupted and the triangular BO_3 building blocks can be arranged in a crystalline unit cell. To date, 2D and 3D crystalline polymorphs that incorporate boroxol groups are only predicted theoretically, although their formation in ambient pressure is crucial to rationalize the B_2O_3 ability to vitrify. Here we present the synthesis of a two-dimensional (2D) B_2O_3 polymorph constituted by boroxol groups bridged by oxygen atoms and arranged in an atomically thin honeycomb lattice. By means of surface science experimental techniques, as well as ab initio calculations [1], we characterized the regular nanoporosity over the mesoscale, the peculiar softness upon isotropic strain, the very weak electronic interaction with the substrate used for growth, Pt(111), and the large band gap in the electronic structure. This discovery adds one member to the family of 2D materials, proves the existence of boroxol-based B_2O_3 crystalline polymorphs and enables the atomic-scale tracking of individual structural units that can be exploited for in-depth studies on the crystalline-vitreous transition of trioxides.

[1] T. Zio et al., Science 390, 95-99 (2025)

645	**Strain-Mediated Lattice Reconstruction Enhances Ferromagnetism in $Cr_2Ge_2Te_6/WTe_2$ van der Waals Heterobilayers**	Franz Herling	Contributed talk (11:00-11:15)

Franz Herling (I1)

(1) Catalan Institute of Nanoscience and Nanotechnology (ICN2)

Van der Waals (vdW) heterostructures enable tailored electronic and magnetic phases by stacking atomically thin layers with pristine interfaces [1–2]. Here, we investigate fully 2D $Cr_2Ge_2Te_6/WTe_2$ heterostructures and identify a strong enhancement of ferromagnetism in $Cr_2Ge_2Te_6$ (CGT). Magnetotransport measurements across multiple devices with WTe_2 thicknesses ranging from monolayer to bulk reveal a robust anomalous Hall effect together with a more than twofold increase of the Curie temperature and substantially enhanced coercive fields. Interface microscopy confirms chemically abrupt vdW interfaces with no detectable interdiffusion, while control experiments rule out processing- or strayfield-induced artifacts. Our experiments and theoretical calculations demonstrate that interfacial charge transfer renders CGT conductive and that proximity-induced lattice distortions in CGT enhance exchange and magnetocrystalline anisotropy [3].
These results establish strainmediated lattice reconstruction as a practical strategy for engineering hightemperature magnetic order in 2D heterostructures [4–6] and clarify that proximity effects in vdW stacks can be governed by modifications within the
magnetic layer itself.

[1] Geim A.K., Grigorieva I.V., Nature, 499 (2013) 419
[2] Novoselov K.S., et al., Science, 353 (2016) aac9439
[3] Herling F., et al., Nano Lett. 26, 16, (2026) 5434–5442
[4] Sierra J.F., et al., Nat. Nanotechnol., 16 (2021) 856
[5] Dong X.-J., et al., Phys. Rev. B, 102 (2020) 144443
[6] Dong X.-J., et al., Phys. Rev. Appl., 12 (2019) 014020

484	**Molecular Motion on Graphene and h-BN: The Role of Surface Polarity and Substrate Coupling**	Anton Tamtögl	Contributed talk (11:15-11:30)

Anton Tamtögl (1) Noah J. Hourigan (1) Jack Kelsall (2) Boyao Liu (2) Anthony Payne (3) Marco Sacchi (3) Philipp Seiler (1)

(1) Graz University of Technology
(2) University of Cambridge
(3) University of Surrey

Molecular adsorption and mobility on two-dimensional materials provide sensitive probes of nanoscale energy dissipation and adsorbate–substrate interactions. In particular, comparing structurally similar but electronically distinct systems such as graphene and hexagonal boron nitride (h-BN) offers a route to understanding how surface polarity, electronic structure, and substrate coupling govern molecular motion [1,2]. Using helium spin-echo (HeSE) spectroscopy, we investigate the nanoscale dynamics of weakly interacting molecules on graphene/Ni(111) and h-BN/Ni(111), where the fast molecular motion is often inaccessible to real-space methods [3]. For benzene, we find thermally activated jump diffusion on both substrates, but with clear differences of the microscopic mechanism: on h-BN/Ni, the motion includes additional confined dynamics such as in-plane rotations and significant contributions from longer-range jumps, whereas on graphene/Ni diffusion is dominated by nearest-neighbour hopping and is more strongly influenced by inter-adsorbate repulsion. Correspondingly, the activation barrier is lower on h-BN, with ≈ 30 meV, and approximately 1.5 times higher on graphene. Water likewise exhibits distinct mobility on the two surfaces, with lower activation energies and stronger rotational–translational coupling on h-BN/Ni(111) than on graphene/Ni(111), revealing a substantially different dynamical regime despite the close structural similarity of the substrates [4].

[1] Unravelling the Epitaxial Growth Mechanism of Hexagonal and Nanoporous Boron Nitride: A First-Principles Microkinetic Model, small 21, 2405404 (2025).
[2] How does intercalation affect the structure and dynamics of bilayer graphene? Carbon 238, 120156 (2025).
[3] Nanoscale Motion of Organic π-Conjugated Molecules: Exploring van der Waals Forces, Friction, and Quantum Effects. Nanoscale Horiz. 10, 3158 (2025).
[4] Understanding water behaviour on 2D material interfaces through single-molecule motion on h-BN and graphene Nat. commun. 16, 10465 (2025).

514	**Fluorophlogopite as a Strong van der Waals Gate Dielectric for MoS_2 Electronics: Breakdown, Electrostatics, and Memory Effects**	Simon Leitner	Contributed talk (11:30-11:45)

Simon Leitner (1) Tibor Grasser (2) Aleksandar Matkovic (1) Egon Pavlica (3) Vadym Tkachuk (3) Axel Verdianu (2) Dominic Waldhör (2)

(1) Montanuniversität Leoben
(2) TU Wien
(3) Univerza v Novi Gorici

Gate dielectrics are a central materials challenge for reliable 2D electronics, where device behaviour is strongly governed by interfacial quality and high-field stability. While hexagonal boron nitride (hBN) is widely used as the benchmark van der Waals dielectric, layered silicates offer an attractive alternative due to their compositional versatility, abundance, and robustness. Here, we present a comparative study of synthetic fluorophlogopite mica (FPh) and hBN as gate dielectrics in MoS_2-based 2D devices.

By combining structural characterization with electrical measurements on capacitor and transistor geometries, we show that FPh sustains markedly higher breakdown fields than hBN, reaching values up to about 10 MV/cm and yielding Weibull statistics consistent with a substantially improved dielectric strength. At moderate gate fields, FPh-based field-effect transistors remain comparable to hBN devices in key figures of merit such as transfer characteristics, threshold voltage, subthreshold swing, and transconductance-based mobility. Dual-gate measurements further give a dielectric constant of about 7 for FPh.

At higher applied fields, however, FPh exhibits an additional functionality absent in hBN: a pronounced and continuously increasing hysteresis that can be tuned by the maximum gate field. We demonstrate field-induced writing of distinct conductance states around zero gate bias and analyse their temporal relaxation. Temperature-dependent hysteresis, Kelvin probe force microscopy, and cross-sectional compositional analysis indicate a mixed mechanism involving both charge trapping and mobile ionic species. These results identify fluorophlogopite as a promising van der Waals dielectric that combines competitive low-field transistor operation with high-field memory-like functionality.

313	**A paradigm shift in sustainable synthesis of MXenes via interfacial phenomena**	Pierluigi Bilotto	Contributed talk (11:45-12:00)

Pierluigi Bilotto (1) Markus Ostermann (1) Marko Piljević (2)

(1) Vienna University of Technology (TU Wien)
(2) AC2T research GmbH

MXenes are a class of two-dimensional materials attracting considerable attention owing to their distinctive physical and chemical properties, which are governed by their surface terminations (Tx). Titanium carbide (Ti3C2Tx) is the most extensively studied MXene, having demonstrated exceptional electrical conductivity, electromagnetic shielding, photonic, and tribological properties.[1] Although upscaling strategies for Ti3C2Tx are actively being explored, a fundamental limitation remains in the synthesis approach. MXenes are conventionally synthesized by employing strong acids (e.g., hydrofluoric acid) to selectively cleave the bonds of the A-group element from their precursor phases (i.e., MAX phases). The handling and use of HF, even in less aggressive synthesis routes such as the MILD method, poses considerable risks to users and the environment, particularly with respect to waste management. Electrochemical synthesis has emerged as a promising alternative for the sustainable production of MXenes; however, its primary limitation has been the achievable yield, which can be severely compromised by the formation of MXene clusters and byproducts on the MAX electrode surface. As a consequence, toxic or hazardous chemicals (e.g., TMAOH) have frequently been employed as synthesis auxiliaries.
Here, we propose a paradigm shift in addressing this challenge. Rather than focusing on electrolyte composition, we demonstrate the critical role of the applied potential waveform, a parameter held constant in previous studies. By employing pulsed voltammetry to apply reverse cathodic pulses, we promote hydrogen evolution at the MAX electrode interface, thereby inducing the formation of surface nanobubbles. These interfacial objects locally modify intermolecular forces (e.g., adhesion) and facilitate the detachment of MXene flakes and byproducts from the MAX electrode into the electrolyte.[2]
The controlled formation of surface nanobubbles enabled operando electrode reactivation, yielding electrochemically synthesized MXene (EC-MXene) with a reduced proportion of F-based terminations and a maximized density of O-based terminations. The exceptional tribological performance of EC-MXene was further validated through an integrated approach combining tribometer measurements, surface analytics, and DFT simulations. These results establish EC-MXene as a benchmark material for sustainable solid lubrication.[3]
In this talk, it will be presented the novel strategy of inducing surface nanobubble formation to regenerate electrochemically active sites on the MAX electrode. The approach opens new avenues for in situ etching synthesis. The implications of this work extend beyond this specific application, with potential relevance to nanobubble–nanoparticle interaction studies, nanocatalysis, and surface termination engineering in two-dimensional materials. Furthermore, the demonstrated application of EC-MXene as a solid lubricant initiates a broader research direction aimed at addressing global challenges in energy consumption efficiency through the development of sustainable lubricants.

P.Bilotto acknowledges Gesellschaft für ForschungsförderungNiederösterreich m.b.H." for support through its FTI PhD Funding Programme(FTI22-D-018).

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2. M. Ostermann, M. Piljevic, E. Akbari, P. Patil, V. Zahorodna, I. Baginskiy, O. Gogotsi, C. Gachot, M. Rodriguez Ripoll, M. Valtiner, P. Bilotto, Small, 2025, 2500807
3. M. Piljevic, M. Ostermann, E. Marquis, S. Schwarz, M. Stöger-Pollach, O. Gogotsi, M. Valtiner, M. Rodriguez Ripoll, C. Gachot, P. Bilotto. Carbon, 2026, 248, 121136

M27 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
289 **P054**	**Liquid phase exfoliated hexagonal boron nitride nanosheet composites towards heat spreader application**	Njomza Isufaj	Poster

Njomza Isufaj (1) Manuel Baumgartner (1) Bernhard C. Bayer (1) Stefan Diebald (2) Manfred Gruber (ATT) Markus Hofer (1) Jan Kotakoski (3) Roman Neuhauser (1) Christian Rentenberger (3)

(1) TU Wien
(2) ATT
(3) Universität Wien

Hexagonal boron nitride (hBN) has emerged as a promising material for various application due to its unique properties, such as high thermal conductivity, electrical insulation, and mechanical strength. Recent advancements in the exfoliation of hBN into nanosheets through liquid-phase exfoliation have opened new opportunities for enhancing heat transport in various systems. This process involves the dispersion of bulk hBN in a solvent, leading to the formation of nanosheets with high surface areas and excellent thermal properties. The high in-plane thermal conductivity of exfoliated hBN enables efficient heat dissipation, essential for improving the performance and longevity of electronic devices. Few-layer 2D-hBN nanosheets are particularly attractive for the use in heat management solutions, including interface material, composites, coating for electronics, energy systems, and advanced materials. Our study demonstrates an effective approach for synthesizing 2D-hBN nanosheets in an environmentally friendly solvent, achieving a high aspect ratio. These nanosheets have potential applications as heat spreaders in electronic devices.

290 **P055**	**ZapTherm: direct in-plane thermal conductivity measurement of 2D material thin films via modified laser-flash-method**	Manuel Baumgartner	Poster

Manuel Baumgartner (1) Njomza Isufaj (1) Bernhard C. Bayer (1)

(1) TU Wien

Two-dimensional (2D) materials such as hexagonal boron nitride (hBN) nanosheets exhibit highly anisotropic thermal conduction pathways, with significantly higher in-plane than out of plane thermal conductivity. This phenomenon increases the difficulty in measuring the in-plane thermal conductivity via conventional one-dimensional (1D) laser flash analysis (LFA) methods, which are commonly used in commercially available lab equipment.
In this work we present, a novel integrated method called “ZapTherm”, which combines spatially resolved thermographic analysis and 2D heat conduction models, to accurately determine thermal diffusivity and thermal conductivity of highly anisotropic composite thin films as well as isotropic bulk materials. The developed measurement method directly determines fundamental thermal quantities without relying on model-based fitting of experimental data, which has been the predominant approach to date. Furthermore, the method is applicable to both free-standing films and substrate-supported samples, enabling the characterization of a wide range of material systems, due to the selective isolation of sample response signal from substrate background.

294 **P056**	**Study of in-situ crystallization and phase evolution of (AlCrTaTiNb)O_2 high entropy oxides in atomic resolution (S)TEM**	Roman Neuhauser	Poster

Roman Neuhauser (1) Bernhard Fickl (1) Alexander Kirnbauer (1) Tushar Gupta (1) Dominik Eder (1) Kimmo Mustonen (2) Clemens Mangler (2) Christian Rentenberger (2) Jani Kotakoski (2) Paul Mayrhofer (1) Bernhard C. Bayer (1)

(1) TU Wien
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High-entropy oxides (HEOs) extend the concept of entropy engineering from metallic alloys to ionic systems, offering a pathway to unprecedented compositionally complex materials with tunable structural and functional properties. Among these, the (AlCrTaTiNb)O2 system serves as a model to study how multiple cations can coexist at random occupation within a single oxide lattice and how such materials crystallize from the amorphous state or phase separate. A key challenge is however to experimentally access this element-specific structural information of such randomly elementary occupied crystalline lattices, that is the defining feature of high entropy materials.
In this work, we leverage suspended monolayer graphene films and ultrathin SiN membranes as ideal substrates for (scanning) transmission electron microscopy ((S)TEM) studies of ultrathin (AlCrTaTiNb)O2 HEOs down to atomic resolution. Using these platforms, we investigate the phase evolution of this archetypical HEO system in two distinct directions: first, by tracking the in-situ crystallization process from the amorphous state, and second, by subjecting the pre-crystallized high-entropy phase to electron beam irradiation to observe its stability and dynamic response.

411 **P057**	**Quantitative study of ion beam-enhanced reactivity of MoS_2**	Francesco Laudani	Poster

Annette Foelske (1) Francesco Laudani (1) Markus Sauer (1)

(1) TU Wien, Analytical Instrumentation Center

Monolayer Molybdenum disulfide (MoS_2) is a two-dimensional transition metal dichalcogenide whose structure is highly sensitive to defect engineering. In our work, we present a quantitative X-ray photoelectron spectroscopy (XPS) investigation of ion beam-enhanced reactivity in monolayer MoS_2, using air oxidation kinetics as a probe of defect-mediated chemical activity. Controlled ion irradiation was employed to introduce a tunable density of lattice defects, including sulfur vacancies. The evolution of surface chemistry upon ambient air exposure was then systematically monitored by XPS. High-resolution Mo 3d core-level spectra reveal a pronounced increase in oxidation rate with increasing ion fluence. Pristine monolayers exhibit minimal oxidation under ambient conditions, whereas irradiated samples show, in comparable timescales, progressive formation of higher oxidation states associated with Mo-O bonding. The oxidation kinetics are expected to follow a defect-density-dependent trend, consistent with vacancy-mediated oxygen adsorption. By correlating ion dose with the fraction of oxidized Mo species, we extract effective reaction rate constants and activation behavior as a function of defect concentration. The data support a model in which ion-induced sulfur vacancies act as primary nucleation centers for oxidation, lowering the kinetic barrier for oxygen chemisorption and accelerating lattice destabilization. At higher fluences, defect clustering further enhances reactivity, leading to spatially non-uniform oxidation and increased chemical heterogeneity. Importantly, the study distinguishes between direct beam-induced chemical modification and subsequent

ambient-driven processes, demonstrating that ion irradiation alters reactivity. These findings provide insight into how controlled ion beam treatment modulates chemical reactivity in molybdenum disulfide. The results have implications for defect engineering and patterning strategies in MoS_2-based electronic and optoelectronic devices, where balancing functionalization and degradation remains critical.

584 P058	**Carbon nanobuds as a 2D hybrid material: topology-constrained synthesis, devices, and outlook**	Reto Stamm	Poster

Raju Lipin (1) Reto Stamm (1) Matthias Vandichel (1)

(1) University of Limerick

Carbon nanobuds - fullerenes covalently bonded to CNTs or to graphene [1] - are hybrid 0D/1D/2D carbons whose bud-substrate junction carries a topologically discrete sp3 defect set by Euler's theorem. In a forthcoming comprehensive survey [2], we critically evaluate the field and identify a persistent imbalance between theory and experiment. Density functional theory predicts Dirac-point modulation, room-temperature magnetism, visible-range nonlinear optical response (with the HOMO–LUMO gap reduced to ~1.70 eV upon C20→C60 fusion [3]), mode-selective phonon scattering, and hydrogen storage; however, most of these predictions remain unvalidated at the level of individual nanobuds.
We organise the outlook along three axes:
Synthesis & functionalisation: approaches including aerosol CVD, solution-phase cycloaddition, electrochemical in situ growth on graphene, and selective covalent chemistry are established, yet deterministic control over placement, size, and density remains elusive.
Characterisation: combined Raman and TEM measurements [4], alongside single-bud STM/STS, can resolve the junction structure, but studies targeting isolated nanobuds are scarce.
(iii) Devices: applications span from commercial transparent conductors (e.g., Canatu NanoBud films for flexible electronics [5]) to a wide range of laboratory-scale prototypes—including low-threshold field emitters (1–2 V μm^{-1} [6]), Li-ion anodes, sensors, thermoelectrics, supercapacitors, and composites—yet lack a unifying materials platform.
Synthesis control emerges as the central bottleneck. We argue that advances in the 2D materials toolbox—such as patterned catalyst islands, van der Waals transfer techniques, and single-bud spectroscopies (STM/STS/PL/Raman)—combined with targeted DFT and molecular dynamics simulations, can bridge the theory–experiment gap. This integrated approach will enable validation of predicted electronic, magnetic, optical, and phononic properties, and support scalable fabrication of device-ready nanobud architectures. Ultimately, this could transform nanobuds from a niche material into a general platform for topology-engineered 2D carbons.

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557 P059	**Adsorption energy prediction and mechanistic analysis of metal atoms on MXene surfaces based on DFT and machine learning**	Wenlong Xi	Poster

Patrick H.-L. Sit (1) Wenlong Xi (1) Zixuan Wu (1)

(1) City University of Hong Kong

MXenes show broad potential as metal-ion battery electrodes due to their tunable surface chemistry and open layered structures. However, traditional density functional theory (DFT) is computationally expensive for systematically screening metal-atom adsorption across diverse MXenes. To overcome this, we propose an efficient machine-learning (ML) framework to predict adsorption energies. Using DFT data, we constructed a cross-element dataset of 90 MXene substrates and 5 metal atoms. We introduce a novel feature-engineering approach that divides MXene surface atoms into three spatial layers, extracting key descriptors like electron affinity and atomic radii. Among four tested ML models, eXtreme Gradient Boosting (XGB) achieved the best predictive performance (MAE = 0.21 eV, R2 = 0.93) with significantly higher efficiency. SHAP analysis identified the electron affinities of the first-layer atoms and the adsorbed metal as the primary factors dictating adsorption energy. Furthermore, we analyzed prototypical high-adsorption MXenes (Sc2NO2 and Y2NO2). Their d-band centers (2.0325 eV and -1.8770 eV) lie closer to the Fermi level, fundamentally explaining their strong adsorption. This study provides a robust, high-throughput screening methodology and critical insights into cross-element adsorption mechanisms for advanced two-dimensional battery materials.

326 P060	**Quantum Capacitance and Stability of $Ti_aV_\beta C_{(a+\beta-1)}$ Double Transition Metal MXenes: A DFT study**	Hamidreza Jouypazadeh	Poster

Hamidreza Jouypazadeh (1) Hayk Zakaryan (1)

(1) Computational Materials Science Laboratory, Center of Materials Science and Nanotechnology, Yerevan State University, Republic of Armenia

Combining high energy and power density makes supercapacitors promising candidates for high-power applications, though their energy density remains lower than that of traditional batteries, largely due to limitations in electrode quantum capacitance. Double transition metal (DTM) MXenes, with their distinctive electronic properties, offer strong potential as electrode materials. In this study, density functional theory (DFT) was applied to evaluate $Ti_aV_\beta C_{(a+\beta-1)}$ MXenes—comprising two to four transition metal layers—for use in electrochemical double-layer capacitors (EDLCs). Phonon dispersion and ab initio molecular dynamics confirmed their dynamic and thermal stability, while elastic constant and Young's modulus analyses demonstrated mechanical robustness superior to mono-transition-metal MXenes. Electronic structure evaluations revealed good conductivity in all but semi-metallic TiVC. Quantum capacitance calculations identified $Ti_2V_2C_3$ as exhibiting the highest integrated quantum capacitance values above 1300 $\mu F/cm^2$ in both ionic/organic and aqueous electrolytes. Comparison with mono-transition-metal MXenes and other known materials underscores the strong promise of these DTM MXenes as next-generation supercapacitor electrode materials.

M28 - Ultrafast and Topological Mechanisms of Ferroic Switching

M28 – Session 1 (Mon 21, 10:30-12:30, Chair: Andrei Pimenov)			
ID	Title	Speaker	Type
574	**Ultrafast phononic switching of ferroic order**	Andrei Kirilyuk	Invited talk (10:30-11:00)

Andrei Kirilyuk (1)

(1) HFML-FELIX, Radboud University

Vibrations of the crystal lattice have a significant impact on the orbital dynamics of the electrons, and through it, on spins. Ultrafast excitation of phonons resulting in drastic repopulation of phononic system was thus shown to be able to modify the fundamental magnetic interactions [1]. And very recently time-resolved X-ray scattering and electron diffraction experiments demonstrated the angular momentum transfer from magnetization to the phonon system, on a femtosecond time scale, dubbed ultrafast Einstein-de-Haas effect [2,3]. It should therefore be possible to realize the opposite process, by changing the lattice and thus controlling the magnetization, on the same time scale - in femtoseconds!
To confirm this, we have recently shown how the resonant excitation of circularly-polarized optical phonons in paramagnetic substrates can permanently reverse the magnetic state of the overlayer [4]. The helicity-dependence of the switching implies that the lattice vibrations excited in the substrate deliver a directional field that pushes the magnetization towards a switched or non-switched state. The nature of such field is however rather unknown and is a topic of debate.
Moreover, a different behaviour, characterized by displacive modification of crystal potentials, is driven by linearly-polarized excitation. The magnetic switching was shown to create very peculiar quadrupolar spatial domain patterns [5], confirming the mechanism. The mechanism appears to be ultimately universal, as observed in variety of systems, not only magnetic ones [6]. The dynamics of the domain formation was shown to proceed via a strongly inhomogeneous magnetic state resulting in a self-organization of magnon-polarons [7] and formation of magneto-elastic solitons.

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339	**Coupled Dynamics of Quantum Orbitals and Quasi-Classical Magnons in Antiferromagnets**	Rostislav Mikhaylovskiy	Invited talk (11:00-11:30)

Rostislav Mikhaylovskiy (1)

(1) Lancaster University

Realisation of quantum information technologies has become a key incentive in material studies and photonics. Orbital 4f states of rare-earth dopants in solids have been identified as one of the most promising agents of quantum computation. Here I discuss how to utilize light waves at THz frequencies to selectively control the low-energy rare-earth states split by the crystal field. As THz photons have meV energy scale, this approach does not require the very low temperatures. Moreover, when embedded into magnetically ordered solids such as 3d metal (e.g. iron, cobalt, nickel) oxides, the rare-earth electronic transitions can strongly hybridise with magnon modes of the ordered 3d spins, leading to spin reorientation phase-transitions, enhanced magneto-optical properties and magneto-electricity. The coupling between the ordered spins and the quantum states of the rare-earth ions mimics the well-known problem of the interface between the quantum and the (quasi)classical systems.
Rare-Earth orthoferrites represent a family of magnetic oxides containing both 3d and 4f (i.e. rare-earth) magnetic ions. The magnetization in these materials mainly arises from the spins of the 3d ions, whereas their orientation is set by the interaction of the 3d spins with the 4f electronic orbitals. While the 3d spins can be considered to behave like quasiclassical (macroscopic) magnetic sub-lattices, the quantum mechanical properties of 4f orbitals cannot be ignored as their populations determine the magnetic state. The interaction between magnons of the ordered spins and the transitions between the rare-earth states, which often form low energy (quasi)doublets, well separated from the higher energy states, is a direct solid-state analogue to the cavity quantum electrodynamics toy model for cooperative behaviour and quantum phase transitions [1].
Using the orthoferrite $TmFeO_3$, we discovered a novel mechanism of nonlinear THz light-spin coupling mediated by Tm^{3+} electronic orbitals. Particularly, resonant pumping the low-energy orbitals changes magnetic anisotropy, which in turn efficiently drives spin motion into nonlinear regime [2]. The strength of the THz-driven anisotropy torque exceeds the Zeeman torque exerted by the magnetic field by at least one order of magnitude [3]. By further increasing the strength of the THz field with the help of custom-made plasmonic THz antennas, we generated anisotropy torques sufficiently high to induce switching between stable antiferromagnetic states [4]. The demonstrated all-coherent spin switching by a THz pulse, involved record low losses of energy of only 1 μeV per spin.The possibility to manipulate the magnetization by THz electric fields opens new prospects for an unprecedented flexibility in the design of recording devices.
Recently we highlighted the influence of the rare-earth ions in the THz response, by comparing the spin dynamics in $ErFeO_3$ with Kramers Er ions and $TmFeO_3$ with non-Kramers Tm ions respectively [5]. Although these materials exhibit very similar properties macroscopically, we observe a remarkable difference in their dynamics across the spin reorientation transition. In $ErFeO_3$, we observe a drastic enhancement of the amplitude of the spin dynamics across the spin reorientation temperature interval, in contrast the response of $TmFeO_3$. We explain this difference by accounting for the strong dynamical coupling of Er electronic transitions and Fe spins and the lack of this coupling between Tm and Fe.
Finally, we present the most recent results on THz-driven dynamics in $YbFeO_3$, which exhibits a spin reorientation transition of the Jahn-Teller type at temperatures below 9 K. In contrast to $TmFeO_3$ and $ErFeO_3$, the orthoferrite $YbFeO_3$ features cross-over of the Yb^{3+} electronic transition with the antiferromagnetic resonance of the iron spins. We show that this energy crossing over results in ultrastrong coupling between quantum Yb^{3+} modes and antiferromagnetic magnons. The origin and properties of this coupling will be discussed, along with our theoretical description We believe that our findings represent a major step in understanding cooperative quantum effects and THz -driven spin dynamics in ultrafast magnetism.

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527	**Diversity of ultrafast laser-induced demagnetization of antiferromagnetic insulators**	Aleksandr Buzdakov	Contributed talk (11:30-11:45)

Aleksandr Buzdakov (1) Ravi Kaushik (1) Nikolai Khokhlov (2) Sergey Artyukhin (1) Alexey Kimel (2)

(1) Istituto Italiano di Tecnologia
(2) Radboud University

Antiferromagnets are promising for spintronics and ultrafast data storage. While femtosecond lasers efficiently quench antiferromagnetic (AFM) order, demagnetization timescales in AFM insulators vary dramatically from picoseconds to nanoseconds. The mechanism behind this variability remains poorly understood. Here, we report the ultrafast melting of AFM order in the insulator Cr_2O_3 compared to the isostructural compound $FeBO_3$. We observe a 100-fold difference: $FeBO_3$ demagnetizes on a sub-nanosecond scale, whereas Cr_2O_3 exhibits rapid demagnetization in under 2 ps. Furthermore, we show this naturally fast process in Cr_2O_3 can be accelerated even further by thermally driving the system above its Néel temperature. Using first-principles calculations and atomistic spin-lattice dynamics, we trace this disparity to how ionic displacements modify spin interactions. The Heisenberg exchange striction in Cr_2O_3 is ten times stronger than in $FeBO_3$. We identify spin-lattice coupling strength as the decisive factor dictating AFM demagnetization timescales, offering a pathway to design faster memory devices.

533	**Topological order parameter switching**	Sergey Artyukhin	Contributed talk (11:45-12:00)

Alessandro Granero (1) Andrei Pimenov (2) Maksim Ryzhkov (2) Sergey Artyukhin (3)

(1) Istituto Italiano di Tecnologia
(2) TU Wien
(3) Quantum Materials Theory, Genova, Italy

Ferroic orders are widely used to encode information in data storage devices and may provide a beneficial way to circumvent Boltzmann tyranny affecting conventional MOSFET memory [1]. However, information writing involves order parameter switching, facilitated by domain nucleation and motion of domain walls across a disordered material, which leads to energy dissipation. Recently, an alternative order parameter switching paradigm has been introduced, where the ordered state tracking the free energy minimum continuously rotates the order parameter direction as the free energy surface is deformed by an external driving [2]. The process is analogous to Thouless pumping and is topologically protected. A related mechanism allows pumping of topological spin textures in space [3].

[1] S. Manipatruni, D. E. Nikonov, I. A. Young, Nature Physics 14, 338 (2018)
[2] L. Ponet et al., Nature 607, 81-85 (2022)
[3] L. Maranzana et al., arXiv:2502.13083

M28 – Session 2 (Tue 22, 10:30-12:30, Chair: Sergey Artyukhin)

ID	Title	Speaker	Type
678	**Dynamics of periodically driven topological magnetic defects**	Maxim Mostovoy	Invited talk (10:30-11:00)

Maxim Mostovoy (1)

(1) Zernike Institute for Advanced Materials, University of Groningen

Low-energy dynamics of magnetic topological defects are governed by collective modes, e.g., center-of-mass coordinates and helicity of skyrmions, as well as the local excitations of the defects with energies below the magnon continuum. The coupling between these modes makes it possible to excite complex, large-amplitude dynamics by periodically oscillating electromagnetic fields and electrical currents. In particular, skyrmions in frustrated magnets with a centrosymmetric crystal lattice can have a local electromagnon mode that can be excited by both electric and magnetic fields and is coupled to the skyrmion chirality. This mode is responsible for the deformation of a moving skyrmion that makes it massive. I will discuss the dynamics of periodically driven topological defects, simulated numerically and described analytically using generalized Thiele equations, which can be used for fast switching of magnetic states and information processing.

451	**All-optical switching of antiferromagnetic domains in ferrotoroidic $LiNiPO_4$**	Shingo Toyoda	Invited talk (11:00-11:30)

Toyoda Shingo (1) Takahisa Arima (1,2) Vilmos Kocsis (3) Istvan Kézsmárki (4) Naoki Ogawa (1) Yasujiro Taguchi (1) Yusuke Tokunaga (2) Yoshinori Tokura (1,5)

(1) RIKEN Center for Emergent Matter Science (CEMS), Wako, Japan
(2) Department of Advanced Materials Science, The University of Tokyo, Kashiwa, Japan
(3) Institut für Festkörperforschung, Dresden, Germany
(4) Center for Electronic Correlations and Magnetism, University of Augsburg, Augsburg, Germany
(5) Tokyo College and department of Applied Physics, The University of Tokyo, Tokyo, Japan

All-optical control of magnetism is key to realizing next-generation opto-spintronic devices that integrate the speed of photonics with the memory functionality of magnetism. In particular, optical control of antiferromagnets is attractive due to their inherently fast spin dynamics and robustness against external perturbations. However, their optical detection and control remain elusive, because conventional opto-magnetic recording and magneto-optical readout techniques rely on net magnetization, which is absent in antiferromagnetic materials.
A potential strategy to overcome this fundamental limitation is to exploit magnetic multipoles other than dipole. In certain multiferroic antiferromagnets, a magnetic toroidal moment, which emerges from vortex-like spin arrangements, serves as a ferroic order parameter. The ferrotoroidic moment can couple to the linear momentum of light, giving rise to the optical magnetoelectric effect (OME), where optical properties depend on the light propagation direction. This mechanism suggests an intriguing possibility of its inverse process, namely IOME effect, in which light propagation direction controls the ferrotoroidic moment.
Here, we experimentally demonstrate the all-optical switching of antiferromagnetic domains in the ferrotoroidic $LiNiPO_4$ by using the IOME effect. This material crystallizes in the centrosymmetric olivine structure and exhibits an antiferromagnetic order below 20.8 K with a ferrotoroidic moment along the b axis. By irradiating intense femtosecond light pulses at 1700 nm which are resonant with the d-d transition of Ni2+ ions, we succeeded in the optical induction of the ferrotoroidic moment and its sign reversal, when light propagation is reversed. We found that this switching process is deterministic, nonvolatile, and efficient enough to switch between single-domain ferrotoroidic states with the opposite ferrotoroidic moment, i.e. between the two time-reversed antiferromagnetic domains.

181	**Multi-cell unit storage based on a multiferroic**	Maksim Ryzhkov	Contributed talk (11:30-11:45)

Maksim Ryzhkov (1) Andrei Pimenov (1) Sergey Artyukhin (2) Alexey Shuvaev (1) Alessandro Granero (2) Maxim Mostovoy (3) Sang-Wook Cheong (4) Anna Pimenov (1)

(1) TU Wien
(2) Istituto Italiano di Tecnologia
(3) University of Groningen
(4) Rutgers University

Recent advances in multiferroic materials offer promising prospects for next-generation memory and data-processing devices. Previous studies [1,2] have shown that rare-earth manganates RMn_2O_5, particularly with R = Gd, are strong candidates for storage applications due to their topologically protected four-state magnetoelectric switching and the efficient electric-field control of this switching.
In this work, we demonstrate that this system enables the realization of a multi-cell storage unit capable of encoding and decoding at least five bits. We show that only two key ingredients are required:
(i) the four-state magnetoelectric switching observed during magnetic-field sweeps, and
(ii) a ferroelectric domain structure in the bulk together with local inhomogeneities (e.g., internal mechanical stresses, compositional variations, or structural defects) that produce a distribution of the spin-flop critical field H_c across different domains.
Thus, the magnetoelectric domains in $GdMn_2O_5$ are not an unwanted bug but an essential feature enabling multi-cell functionality.

[1] L. Ponet, et al., Topologically protected magnetoelectric switching in a multiferroic. Nature 607, 81–85 (2022), doi:10.1038/s41586-022-04851-6
[2] H. Wang, et al., Observation of Universal Topological Magnetoelectric Switching in Multiferroic GdMn2O5. Phys. Rev. Lett. 134, 016708 (2025), doi:10.1103/PhysRevLett.134.016708

544	**Observation of Relativistic Domain Wall Motion in Amorphous Ferrimagnets**	Pietro Diona	Contributed talk (11:45-12:00)

Pietro Diona (1) Sergey Artyukhin (2) Luca Maranzana (2) Giacomo Sala (3)

(1) Scuola Normale Superiore di Pisa
(2) Istituto italiano di Tecnologia
(3) University of Geneva

Domain walls in ferrimagnets and antiferromagnets behave as relativistic sine-Gordon solitons with the spin-wave group velocity setting the ultimate velocity of domain walls and speed of magnetic devices. While this relativistic regime has been achieved in crystalline ferrimagnets, they cannot be routinely integrated in devices. To enable technological breakthroughs, relativistic dynamics must be demonstrated in easy-to-integrate ferrimagnets such as rare-earth – transition-metal alloys. However, this scenario remains elusive due to the inherent magnetic disorder of these materials, their complex spin-wave spectra, and challenges in modeling their ultrafast dynamics. Here, relativistic domain wall motion is demonstrated in amorphous ferrimagnetic GdFeCo devices operated in the proximity of the angular momentum compensation point. The current-induced domain wall velocity saturates within 10% of the spin-wave speed of 2 kms−1, a behavior consistent with relativistic model of domain wall motion. The observation of relativistic dynamics in technologically relevant ferrimagnets opens the way to magnetic devices operating at the ultimate speed limit.

546	**E-field induced unidirectional motion of domain wall in a ferromagnet and time crystals**	Margherita Parodi	Contributed talk (12:00-12:15)

Margherita Parodi (1) Sergey Artyukhin (2) Maxim Mostovoy (3)

(1) Italian Institute of Technology, Genova, Italy
(2) Istituto italiano di Tecnologia
(3) Faculty of Science and Engineering, University of Groningen, The Netherlands

Noncollinear spin textures may break inversion symmetry and induce ferroelectric polarization, giving rise to multiferroicity. Here we study the most basic noncollinear spin texture: a domain wall in a collinear (anti)ferromagnet. The spin chirality of the domain wall is analogous to that in spiral multiferroics and likewise leads to ferroelectric polarization. Here we find that oscillating magnetic and electric fields can drive a unidirectional motion of the magnetic texture, similar to how electrons are transported by the Thouless pump. Furthermore, for certain periods of a driving field, the domain wall demonstrates complex behaviour akin to a time crystal, with the period equal to an integer multiple of the driving periods. The phenomenon arises due to a mismatch between the natural timescale of the domain wall motion and the driving field period.

M29 - Nanomechanical, Electromechanical, Optomechanical and Levitated Systems

M29 – Session 1 (Tue 22, 10:30-12:30, Chair: Albert Schliesser)			
ID	Title	Speaker	Type
306	**Probing the quantum motion of a MHz mechanical resonator with a resonant rf-fluxonium**	Samuel Deléglise	Invited talk (10.30-11:00)

Samuel Deléglise (1)

(1) CNRS

MHz-frequency mechanical resonators are powerful platforms for quantum technologies and tests of fundamental physics, yet efficient control remains challenging due to their low energy scales and the difficulty of coupling them to well-controlled quantum systems at matching frequencies. Here we demonstrate high-fidelity, repeated interactions between a 4-MHz suspended silicon nitride membrane resonator and a resonant superconducting fluxonium qubit. Over the membrane's 6-ms lifetime, the two systems coherently interact more than 300 times. Using the qubit as a stroboscopic spectrometer, we reconstruct the membrane's position-noise spectrum, revealing its thermal occupation, qubit-induced back-action, and the characteristic emission–absorption imbalance. This asymmetry directly reflects the non-commutation of phonon ladder operators, demonstrating the quantum character of the long-lived, massive mode. Because the predicted Diósi–Penrose collapse time is comparable to the membrane's decoherence time, our platform operates in a regime suitable for future interferometric tests of gravity-induced wavefunction collapse.

321	**Carbon nanotube electromechanical force sensor readout through a Josephson travelling wave parametric amplifier**	Patrick Steger	Contributed talk (11:00-11:15)

Patrick Steger (1) Sam Dicker (1) Deepanjan Das (2) Saba Khan (3) Edward Laird (1)

Department of Physics, Lancaster University, Lancaster LA14YB, United Kingdom
Institut Néel, CNRS, Grenoble 38042, France
Department of Applied Physics, Aalto University, Espoo 02150, Finland

Carbon nanotube (CNT) nanoelectromechanical systems are very sensitive to adsorbed mass and external forces, but accurate readout of CNT vibrational motion is essential for these applications. Conveniently, at cryogenic temperatures a suspended CNT single-electron transistor can self-detect its motion, since the conductance depends on the nanotube's displacement. However, the ultimate sensitivity depends on how well this small change in conductance can be amplified and read out.
I will show a readout scheme for a CNT mechanical sensor with a Josephson travelling-wave parametric amplifier (TWPA) as primary gain stage. The TWPA is a near-quantum-limited amplifier mounted inside our dilution refrigerator; we have therefore combined technologies for extremely sensitive force detection and state of the art electronic amplification. To make this work, we operate the CNT as a mixer, with frequencies chosen so that the mechanical motion generates sidebands within the 4-7.5 GHz bandwidth of the TWPA.
With this setup, we have achieved fast and sensitive detection of CNT motion. When the vibrating nanotube is operated in the conventional way, as a mechanical resonator, it is a phase-preserving force detector, and we characterize its force sensitivity. We then operate the device as a self-driving mechanical oscillator, and demonstrate phase-sensitive force detection. These results may be promising for future force microscopes based on nanomechanical resonators and harnessing quantum electronics.

537	**Beyond Internal Resonance: Controlled Energy Transfer in nonlinear Nanomechanical Resonators**	Omid Reza Ranjbar Naeini	Contributed talk (11:15-11:30)

Omid Reza Ranjbar Naeini (1) Jouni Ahopelto (2) Tapani Makkonen (2) Miguel Rubi (3) Clivia Marfa Sotomayor Torres (1)

(1) INL International Iberian Nanotechnology Laboratory, Braga, Portugal
(2) VTT Technical Research Centre of Finland Ltd, Espoo, Finland
(3) Universitat de Barcelona, Barcelona, Spin

Nonlinear mode coupling in micro- and nanoelectromechanical systems (MEMS and NEMS) has been studied extensively because these platforms combine compact size, batch-fabrication compatibility, high reliability, and low power consumption with rich dynamical behavior. In particular, coupled resonators can exhibit energy exchange between interacting modes or neighboring resonators through linear and nonlinear coupling mechanisms. Previous works have established important phenomena such as veering, crossover, internal resonance, chaos, and Hopf bifurcation, significantly advancing the physical understanding of nonlinear interactions in N/MEMS resonators. However, most of these studies have focused on observing, characterizing, or mitigating such phenomena, rather than exploiting them as controllable functional mechanisms to engineer the resurgence time. As a result, a key gap remains in the systematic engineering of dynamic energy transfer and redistribution between coupled modes/ resonators, particularly for applications in communication and computation, where controlled signal flow, recurrence, and energy routing are essential.
In this talk, we address this gap by investigating how nonlinear interactions govern dynamic energy transfer in two nanomechanical systems: intermodal coupling within a single nanobeam and inter-resonator coupling in an engineered array of coupled nanomechanical resonators. We first analyze the nonlinear dynamics of a clamped-clamped Euler-Bernoulli nanobeam, taking into account built-in axial tension, geometric nonlinearity arising from mid-plane stretching, and amplitude-dependent nonlinear damping. Built-in tension is incorporated by means of a tension-dependent shift in the modal frequencies, whereas nonlinearity is described by a cubic modal-coupling term derived from mid-plane stretching. In addition, a phenomenological nonlinear damping term is included to capture amplitude-dependent dissipation. Within this framework, we show that the interplay of these mechanisms gives rise to controlled energy sharing among the fundamental, third-, and fifth-order modes. Importantly, this energy-sharing process depends strongly on the activation force and exhibits a characteristic time-dependent onset, revealing a tunable temporal responce. This behavior is particularly relevant for computational functionality, as the onset and redistribution of modal energy may be harnessed for nonlinear switching and neuromorphic-inspired operations.
We then extend the analysis to a system of nine coupled resonators in order to examine how energy transfer evolves in a larger, designed architecture. In this case, we focus on the dynamics of energy exchange between the first two out-of-plane fundamental modes and show that the transfer dynamics depend sensitively on the resonator design parameters. To capture these effects, we employ a nonlinear model containing both quadratic and cubic nonlinearity,

enabling a broader description of energy redistribution and recurrence in coupled nanomechanical resonators. Our results show that the inclusion of quadratic nonlinearities modifies the recurrence time by altering both the available coupling pathways and the amplitude-dependent frequency shifts. These findings demonstrate that recurrence and energy-flow pathways are not fixed properties of the system but can be engineered through the nonlinear interaction landscape and device design.
The first part of the work identifies how nonlinear dissipation, modal coupling, and forcing conditions determine the onset and timescale of intermodal energy transfer in a single device. The second part shows how nonlinear potential in coupled arrays can reshape redistribution and recurrence dynamics at the multi-resonator level. We show that dynamic energy transfer in nonlinear coupled nanomechanical systems is not merely a secondary consequence of mode interaction, but a controllable physical resource. This makes it a promising mechanism for future communication and computation technologies, including signal routing, logic functionality, information processing, and neuromorphic architectures.

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363	**Surface Loss Reduction by Hyperthermal Annealing in Silicon Nitride Resonators**	Nicola Cavalleri	Contributed talk (11:30-11:45)

Nicola Cavalleri (1) Ariane Giesriegl (1) Silvan Schmid (1) Robert West (1)

(1) TU Wien

Silicon Nitride resonators, due to dissipation dilution and soft clamping, are promising platforms for quantum sensing - even at room temperature. The extremely high $Q \times f$ product allows several coherent oscillations, and by coupling with a cavity they can become fully quantum objects with low phonon occupancy. Given the extremely high aspect ratio used in modern mechanical resonators, surface physics has become one of the limiting factors. In this work, we increase Q with hyperthermal annealing up to 1200C in ultra-high vacuum. With this method, we achieve a $Q \times f = 8 \cdot 10^{14}$ with a phononic crystal membrane, which is, to our knowledge, the highest value reported for this kind of structure to date. To understand the underlying mechanism of surface loss reduction with annealing, we employ techniques such as XPS, FTIR, and ellipsometry, and we propose OH termination as a possible source of mechanical damping.

236	**Fluctuation instabilities via internal resonance in a multimode membrane resonator as a mechanism for frequency combs**	Elke Scheer	Contributed talk (11:45-12:00)

Elke Scheer (1) Orjan Ameye (1) Mengqi Fu (1) Oded Zilberberg (1)

(1) University of Konstanz

In this presentation I will address the possibility to generate an acoustic frequency comb by self-induced parametric coupling of flexural modes in a micron-scale membrane resonator. We detect the flexural modes using an inductive detection scheme [1]. The frequency comb arises as the result of the formation of a limit cycle (LC) following a Hopf bifurcation. We employ a novel pump-noisy-probe technique to record which mechanical excitation sidebands merge at the bifurcation. By thorough theoretical modelling we reveal the mechanism for this comb generation and show that it does not result from locking or synchronizing pre-existing frequencies. Instead, the comb frequency arises from the nonlinear properties of the system and can continuously be tuned by the drive power, similar to the RIFF mechanism [2]. Instead, the comb frequency arises from the nonlinear properties of the system and can continuously be tuned by the drive power [3].

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370	**Quantum-to-classical crossover in a ultra-strongly coupled nanomechanical Rabi system**	Janine Franz	Invited talk (12:00-12:30)

Janine Franz (1) Fabio Pistolesi (1)

(1) Université de Bordeaux, CNRS, LOMA, UMR 5798, Talence France

The ultrastrong coupling regime of the quantum Rabi model has become increasingly accessible in recent years. A particularly promising platform is provided by nanomechanical systems coupled to charge degrees of freedom.
In this work, we consider a quantum mechanical oscillator strongly coupled to a double quantum dot in a regime where the bare energy scales are highly detuned, while the coupling strength ranges from weak to deep-strong relative to the oscillator frequency. Assuming that dissipation is predominantly introduced via the electronic subsystem, we investigate the driven mechanical dynamics across the quantum-to-classical transition. We derive a Lindblad master equation that yields a simple and unified description spanning the fully quantum and classical limits, while also capturing the less understood intermediate crossover regime.

M29 – Session 2 (Tue 22, 16:00-18:00 , Chair: Elke Scheer)			
ID	Title	Speaker	Type
408	**Hybrid Quantum Systems with Ultracoherent Mechanical Resonators**	Albert Schliesser	Invited talk (16:00-16:30)

Albert Schliesser (1)

(1) Niels Bohr Institutet, Københavns Universitet

772	**Dynamical Phase Transitions Across Slow and Fast Regimes in a Two-Tone Driven Duffing Resonator**	Soumya Kumar	Contributed talk (16:30-16:45)

Soumya Kumar (1) Javier del Pino (2) Letizia Catalini (3) Alexander Eichler (4) Oded Zilberberg (1)

(1) Department of Physics, University of Konstanz, 78464 Konstanz, Germany
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(3) Center for Nanophotonics, AMOLF, 1098XG Amsterdam, The Netherlands
(4) Laboratory for Solid State Physics, ETH Zürich, 8093 Zürich, Switzerland

The response of nonlinear resonators to multifrequency driving reveals rich dynamics beyond conventional single-tone theory. We study a Duffing resonator under bichromatic excitation and identify a competition between the two drives, governed by their detuning and relative amplitudes. In the slow-beating regime, where the tones are closely spaced, the secondary tone acts as a modulation that induces dynamical phase transitions between coexisting stationary states. We introduce the cycle-averaged amplitude as an order parameter and map the resulting phase diagram as a function of the drive detuning and amplitude ratio, capturing the pronounced asymmetry observed for blue versus red detuning between the drives in experiment. We link the onset of these transitions to the resonance properties around the nonlinear stationary mode of the system. We apply a two-tone ansatz to this system, for the first time, to provide a comprehensive map of stationary states. Our results provide a framework for controlling driven nonlinear systems, enabling state manipulation, and sensing in nanomechanical, optical, and superconducting circuit platforms.

303	**Photon Blockade in cavity optomechanics at finite drive**	Yvan Briard	Contributed talk (16:45-17:00)

Yvan Briard (1) Clément Dutreix (1) Fabio Pistolesi (1)

(1) Université de Bordeaux, CNRS, LOMA, UMR 5798, Talence France

In cavity optomechanics, it is well established that when the single-photon optomechanical coupling exceeds both the cavity and mechanical damping rates, the optical mode becomes anharmonic. This anharmonicity gives rise to photon blockade, where the frequency difference between the first two excitations prevents a second photon from entering the cavity. An analytical description of this effect exists in the infinitesimal drive limit [1]. Recent circuit QED experiments, which emulate optomechanical systems, operate in a parameter regime where these effects become accessible [2]. In contrast, in the finite- and large-drive regimes, linearization methods successfully describe the system dynamics but fail to capture the nonlinear effects that dominate at low photon numbers.
Here, we develop an analytical framework that incorporates nonlinearities beyond the weak-drive approximation and enables the characterization of photon statistics under finite driving conditions, including resonant, red-sideband, and blue-sideband regimes. Our approach reveals the emergence of additional nonlinear features, such as multiphoton resonance behavior, and identifies parameter regimes where they become significant. Furthermore, we show how these nonlinear interactions can be harnessed to generate near-maximally entangled photon–phonon states, opening perspectives for applications in quantum information processing.

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[2] C. Pott, R. Dekker, S. Deve, E. Strijbis and G. Steele, Strong intrinsic longitudinal coupling in circuit quantum electrodynamics, PRL 134, 153603 (2025)

420	**Toward Multimode Photothermal Sensing**	Dylan Litchfield	Contributed talk (17:00-17:15)

Dylan Litchfield (1) Harmen Smedes (1) Giorgos Markas (2) Fons van der Laan (2) Ewold Verhagen (2) Simon Groeblacher (1) Letizia Catalini (2)

(1) Delft University of Technology
(2) AMOLF

Infrared (IR) detectors are essential for applications including environmental monitoring [1], gas spectroscopy [2], and thermal imaging [3], each imposing distinct requirements on sensitivity, speed, and spatial resolution. While several IR detectors are already commercially available, existing technologies still exhibit fundamental trade-offs [4]: photon detectors offer high sensitivity but require cryogenic cooling, while thermal detectors operate at room temperature but are limited by electrical readout noise, constraining their minimum detectable signal.
Mechanical photothermal detectors offer a promising alternative, transducing absorbed radiation into resonance frequency shifts via thermally induced stress relaxation in a mechanical resonator [5]. When combined with optical readout, this approach largely avoids electrical noise sources, enabling operation near the fundamental thermal fluctuation limit [6], at room temperature.
Here, we explore a new approach to photothermal IR detection based on multi-mode measurement protocols on a highly stressed SiN resonator. We demonstrate that the absorbed radiation induces mode- and position-dependent frequency shifts and compare experimental results with finite element simulations. We envision that this concept could be extended to infer the spatial profile of a spatially distributed source, offering a promising platform for IR imaging applications.

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[3] T. Bamroongshawgasame, X. Zhang and Q. Li, Emerging Trends and Applications in Thermal Imaging Using Infrared Detectors: A Review, IEEE Sens. J. 26, 1520–1532 (2026), https://doi.org/10.1109/JSEN.2025.3635054
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[5] K. Kanellopulos, F. Ladinig, S. Emminger, P. Martini, R. G. West and S. Schmid, Comparative analysis of nanomechanical resonators: sensitivity, response time, and practical considerations in photothermal sensing, Microsystems & Nanoengineering 11, 28 (2025), https://doi.org/10.1038/s41378-025-00879-6
[6] C. Zhang, Z. Louis-Seize, Y. Saleh, M. Brazeau, T. Hodges, M. Turgeon-Roy and R. St-Gelais, Enhanced Bandwidth in Radiation Sensors Operating at the Fundamental Temperature Fluctuation Noise Limit, Nano Lett. 25, 14660–14667 (2025), https://doi.org/10.1021/acs.nanolett.5c03415s

356	**Observing vibration-induced local temperature changes in a silicon nitride membrane under large-amplitude vibration**	Valentin Barth	Contributed talk (17:15-17:30)

Valentin Barth (1) Mengqi Fu (1) Vitali Goussev (1) Elke Scheer (1)

(1) Universität Konstanz

Mechanical properties in MEMS and NEMS are very sensitive to changes in the environment. For the studied membranes, it is known that for example, a global temperature change influences the eigenfrequency [1]. Besides external heating, internal processes due to the vibration (e.g. local friction) could lead to local changes in temperature. Silicon nitride membranes (side length: 450 µm, thickness: 500 nm) are used as resonators, which makes it possible to fabricate thermometers directly on their surface. Local temperature measurements are performed using the thermoelectric effect. Gold and permalloy (Ni81Fe19) can be used to form thermocouples of micrometer size. That provides a sensitivity of 20 µV/K [2]. The system is driven with a piezoelectric actuator and monitored using a digital holographic microscope (DHM), allowing local probing of the vibration [3]. To improve the signal-to-noise ratio of the periodic temperature signal, the measurement is carried out with a lock-in amplifier. The expected signal frequency is twice the drive frequency and is therefore used as the reference for the lock-in measurement. With this setup, sub-millikelvin sensitivity can be achieved.
Measurements are carried out with a strong drive, resulting in vibration amplitudes on the order of hundreds of nanometers and temperature differences of up to 0.5 mK. The signal depends strongly on the thermometer position, both at different locations on the membrane and at positions aside the membrane. In addition, driving strength and vibrational mode also affect the temperature difference. An increase in temperature can also be seen when a neighbouring membrane is vibrating. This coupling between the membranes is confirmed as a change in the frequency response.

[1] F. Yang et al., Sens. Actuators A Phys. 354, 114307 (2023).
[2] F. L. Bakker et al., J. Appl. Phys. 111, 084509 (2012).
[3] G. Coppola et al., Meas. Sci. Technol., vol. 15, 529 (2004)

467	**Resolving Abrikosov Vortex Entry in a Superconducting Nanostring via Cavity Optomechanics**	Tahereh Parvini	Invited talk (17:30-18:00)

Tahereh Parvini (1)

(1) Walther-Meißner-Institut (WMI)

Abrikosov vortices strongly influence dissipation and coherence in superconducting devices, yet their nucleation and pinning dynamics in mesoscopic structures remain difficult to probe experimentally. Here we employ a cavity-optomechanical platform to detect vortex entry in a superconducting aluminum nanostring resonator integrated into a SQUID-terminated microwave cavity. By monitoring the mechanical resonance frequency using displacement-noise spectroscopy at millikelvin temperatures, we observe discrete frequency jumps attributed to individual vortex-entry events. These steps are superimposed on a smooth background consistent with vortex-pinning elasticity in the Campbell regime. From the collective stiffening we extract a Labusch parameter of order $10^{14}\ \mathrm{N\ m^{-4}}$, while individual steps correspond to attonewton-scale force changes and single-vortex pinning energies of $0.1 - 0.4\ \mathrm{eV}$. The stochastic field positions of the jumps across thermal cycles reflect the underlying disorder-defined pinning landscape. Our results demonstrate that nanomechanical cavity-optomechanical devices provide a highly sensitive probe of vortex physics in mesoscopic superconductors and offer a new route to investigate flux-induced dissipation mechanisms relevant for superconducting quantum circuits.

M29 – Session 3 (Wed 23, 16:00-18:00, Chair: Anja Metelmann)

ID	Title	Speaker	Type
506	**Toward sympathetic cooling of a nanoparticle with an ion**	Tracy Northup	Invited talk (16:00-16:30)

Tracy Northup (1)

(1) University of Innsbruck

If two levitated particles are charged and separated by only a short distance, their motion may be appreciably coupled via their Coulomb interaction: cooling just one particle allows the second particle to be cooled as well. This sympathetic cooling is an enabling tool for trapped-ion metrology and computing and has also been demonstrated with nanoparticles in a linear Paul trap [1]. Here, I will discuss prospects for sympathetically cooling a levitated nanoparticle via Doppler cooling of an atomic ion [2]. The proposed experiment builds on our recent demonstration of a nanoparticle stored with a calcium ion in a linear Paul trap [3]. It would allow us to characterize the ion-nanoparticle coupling and understand how it could be applied to future quantum experiments.

[1] D. S. Bykov, L. Dania, F. Goschin, T. E. Northup, Optica 10, 438 (2023)
[2] S. Gupta, D. S. Bykov, T. E. Northup, C. Gonzalez-Ballestero, arXiv:2511:21495 (2025)
[3] D. S. Bykov, L. Dania, F. Goschin, T. E. Northup, Phys. Rev. Lett. 135, 213602 (2025)

234	**Engineering collective motion and light scattering in a nanoparticle tweezer array**	Uros Delic	Contributed talk (16:30-16:45)

Uros Delic (1) Livia Egyed (1) Murad Abuzarli (2) Manuel Reisenbauer (2) Iurie Coroli (2) Benjamin Stickler (3)

(1) TU Wien
(2) University of Vienna
(3) Ulm University

Light is regularly used to trap polarizable objects, such as atoms, molecules, or dielectric nanoparticles. Light is also scattered from them, inducing an interaction mechanism known as light-induced dipolar forces (optical binding). This interaction enables quantum control of the collective motion of arrays of objects, leading to novel opportunities for quantum sensing, quantum metrology, and quantum information science.
In my talk, I will discuss two aspects of cooperative phenomena that arise from tunable light scattering in tweezer arrays of silica nanoparticles. I will show how we can use Floquet-driven, nonreciprocal optical interactions to realize quantum operations on the motion of two trapped objects. Finally, I will present our results on arranging arrays of objects to engineer collective light scattering.

485	**Ultralow loss Meissner- levitated rotor**	Andrea Vinante	Contributed talk (16:45-17:00)

Andrea Vinante (1) Andrea Marchese (2)

(1) CNR-Istituto di Fotonica e Nanotecnologie, Trento
(2) Fondazione Bruno Kessler

I will describe the development and characterization of a spinning rotor based on a Meissner-levitated ferromagnetic microsphere and a synchronous driving technique. We have achieved rotational frequencies above 2 MHz, close to the disintegration limit. We have measured a damping rate well below 1E-6 Hz in vacuum, corresponding to rotational quality factor above 1E13. Finally, we have demonstrated rotor syncronization to a local oscillator. I will discuss potential applications to sensing and to precision measurements relevant to fundamental physics.

309	**Optomechanical Cooling without Residual Heating**	Ciprian Padurariu	Contributed talk (17:00-17:15)

Surangana Sengupta (1) Björn Kubala (1,2) Joachim Ankerhold (1) Ciprian Padurariu (1)

(1) Ulm University, Ulm, Germany
(2) German Aerospace Center (DLR)

Resolved-sideband cooling is a standard technique in cavity optomechanics enabling quantum control of mechanical motion, but its performance is ultimately limited by quantum backaction heating. This fundamental effect imposes a limit on the minimum achievable mechanical phonon number, establishing a finite-temperature floor regardless of the applied cooling strength.
In this talk, we generalize the semi-classical model for optomechanical cooling to describe universal cavity Hamiltonians incorporating both passive and active nonlinearities [1]. As a concrete demonstration, we analyze the simplest circuit optomechanical system that implements a nonlinear drive via a Josephson junction. Our analysis reveals that this active nonlinear drive can eliminate the residual heating backaction. We compare with a series of excellent recent works demonstrating an alternative optomechanical cooling scheme based on passive Kerr-cavity nonlinearities [2,3,4].
By successfully overcoming the finite-temperature floor that limits conventional schemes, our method paves the way for unprecedented quantum control over mechanical systems and establishes the experimental viability of zero-heating optomechanical cooling.

[1] S. Sengupta, et al., Optomechanical Cooling without Residual Heating, arXiv:2511.10318 (2025).
[2] D. Zoepfl, et al., Kerr enhanced backaction cooling in magnetomechanics, Phys. Rev. Lett. 130, 033601 (2023).
[3] N. Diaz-Naufal, et al., Kerr-enhanced optomechanical cooling in the unresolvedsideband regime, Phys. Rev. A 111, 053505 (2025).
[4] L. F. Deeg, et al., Optomechanical backaction in the bistable regime, Phys. Rev. Appl. 23, 014082 (2025).

335	**Magnetically Levitated Systems Approaching the Quantum Regime**	Pietro Oreglia	Contributed talk (17:15-17:30)

Pietro Oreglia (1) Andrea Marchese (2) Daniele Contessi (3) Alessio Recati (4) Andrea Vinante (2) Gianluca Rastelli (4)

(1) University of Trento
(2) IFN--CNR, Fondazione Bruno Kessler
(3) Traverlbrain srl
(4) CNR--INO, Pitaevskii BEC Center

Studying the boundary between quantum and classical physics in macroscopic systems is a central challenge in modern physics. In this context, levitated systems are becoming increasingly important, as they provide excellent isolation and avoid clamping losses, enabling improved quantum control of mechanical motion compared to traditional micro- and nanomechanical resonators. Beyond optical tweezers, magneto-levitated systems based on static superconducting traps that exploit the Meissner effect are particularly promising, as they operate at cryogenic temperatures and exhibit exceptional immunity to dissipative effects. Achieving quantum superposition of massive objects in magnetically levitated systems requires cooling their motion to the quantum ground state. In this talk, I will present a recent proof--of--concept experiment in which we cooled the angular motion of a levitated micromagnet in a superconducting Meissner trap using magnetic feedback. We analyzed the experimental data with a theoretical model tailored to our feedback scheme. Starting from an operating temperature of a few kelvin, we cooled the system down to a few millikelvin. We also discuss how lower temperatures and ground state cooling could be reached through improvements in the performance of the experimental apparatus.
Finally, I will discuss preliminary results from a theoretical study exploring the use of a machine--learning--based strategy (reinforcement learning) to enhance the feedback cooling process. This approach introduces an adaptive agent that controls the feedback in real time, with the ultimate goal of reaching the quantum regime of a massive levitated system.

540	**Non-reciprocal interactions and entanglement between optically levitated nanoparticles**	Benjamin Stickler	Invited talk (17:30-18:00)

Benjamin Stickler (1)

(1) Ulm University

Optically levitating dielectric nanoparticles in ultra-high vacuum, where their motion can be cooled into the deep quantum regime, provides a promising platform for force and torque sensing and for high-mass tests of quantum physics. In this contribution, I will discuss recent results on the coupled dynamics of co-levitated nanoparticles interacting via optical binding and via electrostatic forces. I will show how non-reciprocal interactions [1,2] and mechanical entanglement [3,4] between two particles can be generated and observed by controlling the light fields suspending them.

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[2] Reisenbauer, Rudolph, Egyed, Hornberger, Zasedatelev, Abuzarli, Stickler, and Delić, Nat. Phys. 20, 1629 (2024)
[3] Rudolph, Delić, Aspelmeyer, Hornberger, and Stickler, Phys. Rev. Lett. 129, 193602 (2022)
[4] Rudolph, Delić, Hornberger, and Stickler, Phys. Rev. Lett. 133, 233603 (2024)

M29 – Session 4 (Thu 24, 16:00-18:00, Chair: Silvan Schmid)

ID	Title	Speaker	Type
495	**Overcoming Fundamental Design and Noise Limitations of MEMS Resonators**	Daniel Platz	Invited talk (30 min.)

Daniel Platz () Ioan Ignat (1) MinHee Kwon (1) Christoph Schallert (1) Ulrich Schmid (1) Andre Gesing (1)

(1) TU Wien

Microelectromechanical systems (MEMS) are a success story of modern engineering with billions of MEMS sensors in automotive, consumer and industrial use. However, despite decades of research, limitations persist. One fundamental aspect of MEMS sensor performance centers on how a MEMS resonator interacts with its environment. These interactions can be highly complex and modelling them has been restricted to slender geometries limiting the available design space. A challenging example is the interaction with a liquid environment which is essential for bio- and fluid sensing. Conventional beam resonators suffer from quality factors well below 100 in liquids severely degrading sensitivity. By developing modeling methods that move beyond the beam paradigm toward non-slender plate geometries while retaining computational efficiency, we show that MEMS plate resonators reach quality factors above 300 in water representing a significant advance for bio and liquid sensing. A second fundamental limitation in MEMS is noise. Cavity optomechanics has shown that thermal and measurement noise can be reduced to the ultimate quantum-mechanical limits. Yet real-world applicability remains constrained by bulky optical components and cryogenic requirements. Our work pursues two strategies to bring these concepts into a scalable MEMS platform. First, the established vacuum-gap capacitor platform for quantum electromechanics is advanced toward higher operating temperatures through niobium as a superconducting material. Second, the electromagnetic cavity is replaced by a mechanical GHz surface acoustic wave (SAW) resonator fabricated with standard MEMS processes. We demonstrate parametric coupling between this SAW mode and low-frequency flexural cantilever modes establishing a mechano-mechanical analogue of cavity optomechanics on a single silicon chip. Our findings demonstrate that MEMS still have not reached their limits and have great potential for groundbreaking future applications.

ID	Title	Speaker	Type
89	**Efficient mapping and tracking the properties of micromechanical resonators using phase-lock loops with closely-spaced frequencies**	Menno Poot	Contributed talk (15 min.)

Menno Poot (1) Samer Houri (2) Agnes Zinth (3)

(1) Münster University
(2) Imec
(3) TU Munich

Understanding the dynamical behavior of micro- and nano-mechanical systems (MEMS and NEMS) is essential in a wide variety of applications ranging from nonlinear dynamics to quantum technologies. Hence, it is important to be able to precisely monitor the mechanical properties of MEMS and NEMS devices. In this contribution, we show how to track and spatially map various properties of a mechanical resonator, specifically frequency shift, linewidth, and nonlinearity, by aptly choosing three closely-spaced drive frequencies and using phase-locked loops (PLLs). This technique tracks changes in the system faster and more efficiently, without the need for repeated frequency sweeps of the oscillator response, simply by employing three phase-locked tones.
The resonator we use to demonstrate our technique is a hexagonal micromechanical membrane made from high-stress silicon nitride (SiN) whose motion is read out using an interferometric setup. The fundamental out of plane mode around 1.7 MHz has a linewidth of only 22 Hz. Still, by selecting different setpoints, three PLLs can be locked to this single narrow resonance. In the event of a frequency shift, all three locked frequencies will move in unison. On the other hand, a change in linewidth will only change the separation between the two outer ones. Also, a change in the Duffing nonlinearity has a distinct signature. We demonstrate that the frequency and linewidth can be tracked during a large temperature ramp, where a regular network analyzer measurement would be way too slow. By scanning the membrane underneath the laser spot, spatial maps of feedback-induced effects are measured. The results are further improved by constructing an estimator. Finally, when adjusting the driving power also the Duffing nonlinearity is determined.
Our very robust method allows to investigate a plethora of unintentional features of our resonator like sign changes, thickness variations, or particles on the membrane. Thus, it enables a fast characterization, spatial mapping and monitoring of properties of changing micro- and nano-mechanical systems in real time.

ID	Title	Speaker	Type
239	**Optimizing highly symmetric 2D Nanomechanical resonators beyond band-gap Phononic crystals**	Mohit Kumar	Contributed talk (15 min.)

Andreas Isacsson (1) Mohit Kumar (1)

(1) Chalmers University of Technology

Two-dimensional (2D) ultracoherent nanomechanical resonators are promising platforms for room-temperature quantum sensing, precision metrology, and cavity optomechanics, but their performance is often limited by mechanical dissipation, large effective motional mass, and insufficient optomechanical coupling. In this work, we demonstrate that highly symmetric 2D nanomechanical resonators can achieve high quality factors by exploiting localized modes beyond the conventional phononic band-gap mechanism in highly stressed silicon nitride membranes. We develop a hybrid inverse-design strategy that combines Bayesian optimization with topology optimization to efficiently search complex geometries and identify structures with favorable modal properties. In particular, this hybrid strategy is used to maximize the dissipation dilution factor while simultaneously reducing the effective motional mass, two key parameters for high-performance resonator design. Our results show that highly symmetric structures can reach performance metrics comparable to those of band-gap-based phononic crystal resonators, while offering an alternative route for engineering ultracoherent mechanical modes. These findings highlight the potential of highly symmetric membrane architectures for the realization of low-loss, low-mass, and optomechanically favorable resonators for future sensing and quantum technologies.

261	**Tuning of on-chip mechanical resonators on SiC by bending-induced stress**	Heiko Weber	Contributed talk (15 min.)

Alexander D. Fuchs (1) André Hochreiter (1) Heiko B. Weber (1)

(1) Friedrich-Alexander-Universität Erlangen-Nürnberg

Silicon carbide (SiC) is a material that could advance the field of nanomechanics thanks to its exceptional low internal damping. Even more exciting is the prospect of hybridising mechanics with the spin degrees of freedom of colour centres such as VSI, which opens up additional possibilities for quantum sensing and quantum communication.
However, the challenge lies in matching the frequency of a nanomechanical resonator with that of a spin when the resonance is as narrow as a single Hertz. We present recent experiments and results in continuation of high-quality-factor resonator studies [1,2] where the frequency of a monolithically fabricated single-crystal resonator is continuously tuned from approximately zero stress to more than 200 MPa. This analysis became possible by a thorough validation between simulation and experiment. The result of the first experiments is a 250% increase of the fundamental eigenfrequency and, simultaneously, a five-fold boost of the mechanical quality factor.

[1] A. Hochreiter, F. Groß, M.-N. Möller, M. Krieger, and H. B. Weber, Electrochemical etching strategy for shaping monolithic 3D structures from 4H-SiC wafers, Scientific Reports 13 (2023), DOI:10.1038/s41598-023-46110-2.
[2] A. Hochreiter, P. Bredol, F. David, B. Demiralp, H. B. Weber, and E. M. Weig, Monolithic 4H-SiC nanomechanical resonators with high intrinsic quality factors, Physical Review Applied 24 (2025), DOI:10.1103/vclj-v8qx.

299	**UV-Vis-NIR Complex Refractive Index Characterization of Silicon Nitride Thin Films**	Thomas Mathias Tropper	Contributed talk (15 min.)

Thomas Mathias Tropper (1) Sebastian Alberti (1) Ariane Giesriegl (1) Kostas Kanellopulos (1) Silvan Schmid (1)

(1) Institut für Sensor- und Aktuatorsysteme, TU Wien

Silicon nitride (SiN_x) is a widely used material in nanomechanics and integrated photonics due to its favorable mechanical and optical properties. In photonics, it serves as a low-loss platform for optical waveguides owing to its low extinction coefficient $k(\lambda)$ in the infrared (IR).
Conventional determination of the complex refractive index $\tilde{n}(\lambda)$ relies on measurements of transmittance T and reflectance R, which are interpreted using optical models to extract $n(\lambda)$ and $k(\lambda)$. Absorptance is often inferred as $A = 1 - T - R$. In the low-loss regime, A becomes very small and difficult to distinguish from scattering contributions and measurement noise, limiting the reliability of such extraction methods.
Here, we use tensile-stressed SiN_x nanomechanical resonators as photothermal sensors. Monochromatic UV–NIR illumination induces heating proportional to optical absorption, leading to thermal expansion and a corresponding shift in resonance frequency. This shift scales with absorptance, $\Delta f_0/f_0 \propto A(\lambda)$, enabling an alternative route to quantify optical absorption. Combining this with transmission measurements improves the robustness of the determination of the complex refractive index, in particular the extinction coefficient $k(\lambda)$.

434	**Neuron-Inspired Computing via Phonon–Cavity Dynamics in Coupled Microelectromechanical Drum Resonators**	Theresa Farah	Invited talk (30 min.)

Theresa Farah (1,2) Loic Flis (1,2) Bahram Djafari-Rouhani (2) Yan Pennec (2) Xin Zhou (1,2)

(1) CNRS
(2) IEMN, University of Lille

Reservoir computing is a bio-inspired computational paradigm that exploits the intrinsic dynamics of complex systems for temporal information processing. For any physical element to perform reservoir computing, it requires to have at least features of (1) nonlinearity and (2) fading memory.
Microelectromechanical resonators, owing to their inherent nonlinearity and transient states, constitute an attractive platform for reservoir computing while offering the ability to integrate of sensing and computing within a single hardware device [1-2].
Here, we present our recent work on the experimental demonstration of reservoir computing in a double-drum electromechanical system [3–5]. Within the framework of phonon–cavity electromechanics, a virtual neural network is mapped onto two capacitively coupled drum resonators by modulating the pump force to induce the required nonlinearity via sideband pumping of the phonon cavity. This pump tone generates nonlinear dynamics in the energy transfer between the two resonators, enabling reservoir computing functionality. To enhance the memory capacity of the system, we exploit not only the intrinsic transient dynamics of the mechanical resonators but also implement a time-delayed feedback loop, which establishes coupling between the current and past states for temporal information processing.
The performance of the resulting neural network is evaluated using both parity-benchmarks and normalized auto-regressive moving average (NARMA) benchmarks through training and prediction tasks. Furthermore, to demonstrate the integration of sensing and computing within this double-drum system, one of the coupled resonators is used as the input sensing channel, while the other serves as the computational node for training and readout. This new, neuron-inspired computing scheme can easily be extended to other multimode coupling platforms, such as mechanically coupled resonator arrays and optomechanical systems.

[1] G. Dion, et al., J. App. Phys. 124,152132 (2018).

[2] X. Guo, et al. Microsyst Nanoeng 10, 84 (2024).
[3] X. Zhou, et al. Nano Letters, 21(13), 5738-5744 (2021)
[4] A. Pokharel, et al. Nano Letters 22(18), 7351–7357 (2022)
[5] T. Farah, et al, arXiv:2601.02617v3, accepted by Microsystems & Nanoengineering (2026)

M29 – Session 5 (Fri 25, 10:30-12:30, Chair: Gianluca Rastelli)

ID	Title	Speaker	Type
466	**Nonlinearity as a Resource for Optomechanics**	Anja Metelmann	Invited talk (10:30-11:00)

Anja Metelmann (1)

(1) Karlsruhe Institute of Technology

Nonlinearities are a fundamental feature of many physical systems and can serve as a powerful resource when properly controlled. In optomechanics, where light interacts with mechanical motion, they provide new opportunities for exploring regimes beyond those described by linear dynamics. In this talk, we present how engineered nonlinearities can be harnessed in cavity optomechanical systems to access new behavior at low excitation levels and to modify the interaction between light and mechanical motion. We demonstrate that nonlinearity enables the observation of dynamical effects in the few-excitation regime and can influence the efficiency of optomechanical cooling. In particular, we show that nonlinear cavities can enhance cooling performance compared to their linear counterparts. These results illustrate how nonlinearity can be used to extend the range of accessible phenomena in optomechanical systems, with relevance for quantum science and precision measurements.

ID	Title	Speaker	Type
223	**Experimental Quantification of Nonlinear Mode-Coupling in Nanomechanical Resonators using Multi-tone Excitation**	Chris Wattjes	Contributed talk (11:00-11:15)

Farbod Alijani (1) Zichao Li (1) Richard Norte (1) Peter Steeneken (1) Chris Wattjes (1) Minxing Xu (1)

(1) TU Delft

Nonlinear interactions in resonant systems play a key role in many physical and engineering phenomena, but experimentally determining their coupling strengths remains challenging, particularly in multimode structures. We introduce a frequency-domain framework that enables direct experimental quantification of nonlinear modal couplings in multi-mode nanomechanical resonators using tailored multi-tone excitation. In our approach, dual-tone drives placed near selected resonances, combined with additional probing tones at higher-order modes, generate sideband responses that isolate specific modal interactions. By applying an inverse reconstruction procedure to these sidebands, we extract the corresponding nonlinear coupling strengths and reconstruct fully experimental, device-specific nonlinear reduced-order models.
Applied to high-stress Si_3N_4 nanostrings, the method enables quantification of linear parameters, Duffing nonlinearities, and pairwise coupling coefficients across the first five vibrational modes. The resulting experimentally derived models shows excellent agreement with finite-element-based nonlinear models, demonstrating both the accuracy and robustness of the approach.
Because the method relies purely on controlled nonlinear mixing, it does not require operating in internal-resonance conditions or performing time-domain ring-down measurements. The procedure scales naturally to higher-order interactions and can be extended to systems exhibiting quadratic or hybrid couplings. Overall, this framework provides a general, data-driven route for characterizing complex nonlinear interactions in micro- and nanoscale resonant systems.

A preprint detailing our approach can be found on: https://arxiv.org/html/2604.13920v1

ID	Title	Speaker	Type
53	**Non-reciprocal interactions between a mechanical oscillator and an atomic spin system**	Gian-Luca Schmid	Contributed talk (11:15-11:30)

Gian-Luca Schmid (1) Philipp Treutlein (1) Andreas Weber (1) Alvaro de Melo (1)

(1) Department of Physics, University of Basel

Non-reciprocal interactions violate the action-reaction symmetry of Newton's third law, giving rise to phenomena such as amplification, synchronization, and spontaneous parity-time symmetry breaking. In quantum systems, non-reciprocal interactions have recently attracted significant interest as a new tool to engineer functionality, with potential for sensing and signal processing applications. Here we report experiments on non-reciprocal interactions in a hybrid mechanical-atomic system coupled by light. We observe spontaneous coupled oscillations, two-mode squeezing dynamics, limit cycles and phase synchronization of the two systems.

ID	Title	Speaker	Type
531	**Nanomechanics in the atomically thin amorphous limit**	Liga Jasulaneca	Contributed talk (11:30-11:45)

Liga Jasulaneca (1) Farbod Alijani (1) Artem Grebenko (2) Alberto Martín-Pérez (1) Prertahn Munireternam (2) Hongji Zhang (2) Barbaros Özyilmaz (2) Makars Šiškins (3)

(1) Delft University of Technology
(2) National University of Singapore
(3) University of Southampton

Two-dimensional nanomechanical resonators have been studied mainly in crystalline materials, leaving the atomically thin amorphous limit largely unexplored. Here we study this regime in suspended nanodrum resonators made from monolayer amorphous carbon (MAC), an intrinsically disordered two-dimensional membrane. Using optothermal actuation and interferometric readout, we resolve thermomechanical motion, driven resonances, and multimode spectra in vacuum. The measured devices show broad distributions in resonance frequency and quality factor, consistent with heterogeneous stress and disorder in the amorphous membrane. Under stronger drive, the resonators display rich nonlinear behavior, including hardening, softening, and

mixed Duffing response, as well as nonlinear damping and parametric spectral features. In some drums, the observed responses and mode structure are further consistent with intermodal coupling and possible internal resonance. Our results establish MAC as a promising model system for probing disorder-sensitive nonlinear nanomechanics in the two-dimensional amorphous limit.

284	**Frequency Stability of Graphene Nonlinear Parametric Oscillator**	Enise Kartal	Contributed talk (11:45-12:00)

Enise Kartal (1) Oriel Shoshani (2) Elena Botnaru (1) Alberto Martín-Pérez (1) Tomás Manzaneque (1) Farbod Alijani (1)

(1) Delft University of Technology
(2) Ben-Gurion University

High-frequency stability is a defining metric for the performance of nanomechanical resonators in advanced sensing and timekeeping applications. While 2D materials like graphene offer extreme miniaturization, high mechanical compliance, and high responsivity, these properties make them highly susceptible to nonlinearities that degrade frequency stability. Here, we demonstrate that graphene parametric oscillators unlock an alternative nonlinear operating regime, in which short-term frequency stability is enhanced by strong nonlinear damping.
To trace the nonlinear dynamics of graphene nanomechanical resonators, we operate them in a closed loop via a phase-locked loop (PLL). We experimentally demonstrate that parametric oscillations in the post-bifurcation regime yield a lower Allan deviation at fast integration times compared to standard Duffing oscillations at equivalent drive amplitudes. We attribute the physical origin of this improvement to strong nonlinear damping inherent to parametric oscillators, a mechanism that effectively suppresses amplitude-to-frequency noise conversion even at large operational amplitudes.
To validate our experimental findings, we present a minimalistic theoretical model that captures the observed phase diffusion dynamics. The model confirms nonlinear damping as the dominant mechanism governing phase noise reduction. Ultimately, while traditional sensing views nonlinearities as detrimental, these results provide a new framework for operating highly compliant nano-, electro-, and optomechanical systems, highlighting how nonlinear damping can be harnessed to push precision sensing beyond the conventional limits of graphene oscillators.

Kartal, E., Shoshani, O., Botnaru, E., Martín-Pérez, A., Manzaneque, T., & Alijani, F. Frequency Stability of Graphene Nonlinear Parametric Oscillator. Nano Letters. https://doi.org/10.1021/acs.nanolett.6c00581

369	**Tuning and Mapping of Two-Tone Optomechical Instability up to the Physical Limits**	Marco Dicosta	Invited talk (12:00-12:30)

Marco Dicosta (1) Eddy Collin (1) Alexander Delattre (1) Andrew Fefferman (1) Laure Mercier de Lépinay (2) Mika Sillanpää (2)

(1) Neel, CNRS
(2) Aalto University

Measurement back-action imposes a fundamental limit on the precision of interferometric measurements of mechanical motion, setting the standard quantum limit (SQL) for continuous opto-mechanical detection. Back-action evading (BAE) measurement schemes provide a route to surpass this limit by selectively measuring a single quadrature of motion, rejecting all back-action noise onto the other one. Practical implementations are often limited by tuning capabilities and ultimately intrinsic instabilities.
It has been theoretically shown that two-tone driving schemes enables one to perform BAE measurements [1]. Further experiments demonstrated the effect using microwave opto-mechnanics at low temperatures [2]. A recent work has addressed the issue of the two-tone instability, studying the dynamic range accessible to BAE optomechanical
measurements [3]. This work was both experimental and theoretical, but the agreement between the two, even phenomenologically correct, shows discrepancies. Here we demonstrate very good agreement between theory and microwave opto-mechanics experiments, starting from a complete Hamiltonian that incorporates all instrumental imperfections. We observe the effect of mistunings on the system in all possible parameters, including the power imbalance of the pumps which was not addressed before. We also study the physical limit of tuning for BAE measurements, showing that this limitation is a resultant of the intrinsic noise inside the system.

[1] A A Clerk, F Marquardt, and K Jacobs. Back-action evasion and squeezing of a mechanical resonator using a cavity detector. New Journal of Physics, 10(9):095010, Sep 2008.
[2] J. B. Hertzberg, T. Rocheleau, T. Ndukum, M. Savva, A. A. Clerk, and K. C. Schwab. Back-action-evading measurements of nanomechanical motion. Nature Physics, 6(3):213–217, Dec 2009.
[3] Itay Shomroni, Amir Youssefi, Nick Sauerwein, Liu Qiu, Paul Seidler, Daniel Malz, Andreas Nunnenkamp, and Tobias J. Kippenberg. Two-tone optomechanical instability and its fundamental implications for backaction-evading measurements. Physical Review X, 9(4), Oct 2019.

M29 – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
149 **P061**	**Towards a mechanical nonlinearity in the few-phonon regime based on the Casimir force**	Matthijs de Jong	Poster

Matthijs de Jong (1) Johannes Fink (1)

(1) Institute of Science and Technology Austria

Nanomechanical resonators have shown long lifetimes (Q > 10^9) and long coherence times, which makes them promising for quantum information applications as memories or transducers. However, their linear behaviour limits which quantum operations can be performed: An amplitude-dependent nonlinearity is necessary to realize a complete set of quantum gates. Recently, nanomechanical resonators have been shown to behave nonlinearly in the few-phonon regime by hybridizing to a superconducting qubit or double quantum dot in the strong or ultrastrong coupling regime. Here, I propose that the same could be achieved without coupling to any external quantum system via the Casimir force that exists between closely spaced objects.

474 **P062**	**Two-Level-System Induced Frequency Shift in AlN-based SAW Resonators at Ultra-Low Temperatures down to 10 mK**	Christoph Anton Schallert	Poster

Christoph Anton Schallert (1) Viktor Wahler (1) Masiar Sistani (1) Walter Weber (1) Daniel Platz (1) Ulrich Schmid (1)

(1) TU Wien

Surface acoustic wave (SAW) resonators based on aluminum nitride (AlN) operating in the gigahertz frequency range are promising platforms for hybrid quantum systems. At a temperature of 10 mK, the SAW resonator is governed by quantum noise, and the internal loss can be attributed to phonons coupling to two-level-systems (TLS), which arise from tunneling states linked to elastic and electric fields. One straightforward approach to determining TLS losses is to measure the resonance frequency shift as a function of temperature. However, the microscopic origin of TLS losses in AlN remains unresolved, particularly below $T = hf/2k_B$, where precise thermalization---and thus accurate temperature control---of the SAW resonator becomes challenging. Here, we present the resonance frequency shift of an AlN-based SAW resonator designed for 4 GHz operation, measured across temperatures from 10 to 700 mK. Our analysis reveals a nonlinear shift in the resonance frequency $\Delta f_r = f_r(T) - f_r(T \to 0)$, ranging from -0.040 to +0.187 MHz around $f_r(T \to 0) = 4274.794$ MHz, with a minimum near T = 100 mK. This result is in good agreement with the standard theoretical model for TLS, which predicts a minimum at $T = hf_r/2k_B = 103$ mK. Furthermore, the extracted data points fit well to the TLS model when including a frequency offset of -21 kHz as the temperature approaches 0 K ($T \to 0$). Finally, this analysis yields a TLS-related internal quality factor of $Q_{\mathrm{i,TLS}} = 7237$. Our results demonstrate the presence of TLS-related losses in AlN-based SAW resonators operating at low-gigahertz frequencies and millikelvin temperatures. Moreover, precise temperature control of the SAW resonator enables accurate extraction of $Q_{\mathrm{i,TLS}}$. This refinement in measurement precision is particularly significant, as TLS-related losses are highly relevant in the single-excitation limit and, consequently, for quantum applications.

515 **P063**	**Squeezing in Coupled Nanomechanical Resonators**	Xin Zhou	Poster

Loic Flis (1) Theresa Farah (1) Francesco Massel (2) Xin Zhou (1)

(1) CNRS, IEMN
(2) Department of Science and Industry Systems, University of South-Eastern Norway

Coupled nanomechanical systems provide versatile experimental and theoretical platforms for exploring classical-to-quantum analogies, nonlinear dynamics, and quantum phenomena. One particularly important topic is the generation of squeezed states in mechanical oscillators, where quadrature fluctuations are reduced below the standard quantum limit [1-2]. In this work, we experimentally demonstrate dissipative squeezing in a system of two capacitively coupled drum electromechanical resonators by simultaneously pumping the red and blue sidebands of one resonator. By monitoring the quadrature variances of both coupled mechanical modes at room temperature, we observe signatures of steady-state squeezing. We further analyze the achievable minimum squeezing level and elucidate its underlying mechanism by comparing it with the fundamental limits imposed in conventional parametric pumping schemes.

[1] A. Vinante et al., Phys. Rev. Lett. 111, 207203 (2013)
[2] E. E. Wollman, et al., Science 349, 952 (2015).

594 **P064**	**Raman Spectroscopy of Single Levitated Nano Particles in a Paul Trap**	David Jakob	Poster

David Jakob (1) Markus Weber (1) Andreas Schell (1)

(1) Johannes-Kepler-Universität Linz

Paul traps offer exceptional control over charged micro- and nanoparticles, making them ideal platforms for non-destructive optical characterization. In this work, we present a setup combining a Paul trap with Raman spectroscopy to study nanoparticles in levitation. Individual particles are loaded into the trap and confined through electric fields, allowing extended interrogation times without substrate contact, preparation artifacts, or contamination from the environment. Raman spectra are acquired to characterize the chemical composition and molecular structure of the trapped particles. This approach demonstrates the potential of levitated single-particle platforms for label free chemical identification of airborne and environmentally relevant particles. The mechanical behaviour of the confined particles is systematically characterized to ensure stability and determine oscillation amplitudes, improving the consistency of the acquired spectra. In the future, we plan to perform additional measurements of the nanoparticles' mass [1], and to control the temperature as well as the surface chemistry of the particles in order to implement a chemical nanoreactor [2].

[1] F. Ricci, M. T. Cuairan, G. P. Conangla, A. W. Schell, and R. Quidant. Accurate mass measurement of a levitated nanomechanical resonator using corona discharge. Nano Letters, 19(10):6711-6715, 2019.
[2] F. Ricci, M. T. Cuairan, A. W. Schell, E. Hebestreit, R. A. Rica, N. Meyer, and R. Quidant. A chemical nanoreactor based on a levitated nanoparticle in vacuum. ACS Nano, 16(6):8677-8683, 2022.

755 **P065**	**Optomechanical Cavities as Physical Reservoirs: Dynamical Regimes and Noise Resilience from a Coupled-Mode Theory Perspective**	Samaneh Moeini	Poster

Samaneh Moeini (1)

(1) International Iberian Nanotechnology Laboratory - INL

M30 - Focused Beam Technologies for Functional Nanodevices

M30 – Session 1 (Wed 23, 10:30-12:30)			
ID	Title	Speaker	Type
796	**Direct-Write Nanofabrication of Functional Devices Using Focused Particle Beams**	Robert Winkler	Invited talk (10:30-11:00)

Robert Winkler (1)

(1) Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology , 8010 Graz, Austria

126	**3D Nanomagnetism Enabled by Focused Electron/Ion Beams**	Amalio Fernandez-Pacheco	Invited talk (11:00-11:30)

Amalio Fernandez-Pacheco (1)

(1) TU Wien

The extension of nanotechnology into three dimensions presents compelling opportunities to explore emergent physical phenomena while enabling the realization of next-generation 3D device architectures for future computing. At the same time, this transition introduces substantial challenges, requiring advanced nanofabrication strategies that surpass the limits of conventional lithographic techniques.
In this presentation, I will highlight our recent advances in nanoscale 3D printing based on focused electron-beam-induced deposition. This platform, developed within our group, allows for the precise fabrication of arbitrary three-dimensional nano-geometries, providing a versatile route to experimentally access phenomena that arise specifically from three-dimensionality. Particular emphasis will be placed on applications in nanomagnetism and superconductivity.
I will present representative examples of 3D nano-devices that reveal these novel effects, including the stabilization of complex topological spin textures and defects, the formation of topological stray fields in free space, the manipulation of domain wall motion via strong 3D geometric gradients, unconventional magnetotransport signatures linked to intricate demagnetizing fields, and the reconfigurable behavior of superconducting vortex circuits.
Furthermore, I will discuss complementary experimental and computational methodologies developed in our group, such as dark-field magneto-optics, which enable detailed characterization of these systems. In addition, we will compare key differences between fabrication approaches based on focused electrons and ions, highlighting their respective advantages and limitations for 3D nanostructuring. Finally, I will outline prospects for 3D nanostructures in emerging areas including spintronics, magnonics, and fluxonics.

137	**Growth of nanotips by FEBID, and their use in Biology, Materials Science and Nanomagnetism**	Jose Maria de Teresa	Contributed talk (11:30-11:45)

Jose Maria de Teresa (1) Alix Tatiana Escalante-Quiceno (1) Lucía Herrer (1) César Magén (1) Soraya Sangiao (1)

(1) Instituto de Nanociencia y Materiales de Aragón (CSIC-Universidad de Zaragoza)

Investigations in fundamental science require advanced tools. In particular, the field of Nanoscience uses scanning electron and ion microscopes that allow imaging and patterning materials with resolution in the range of 1 nm [1, 2]. These microscopes are known as the Scanning Electron Microscope (SEM) and the Focused Ion Beam (FIB). Besides, Nanoscience studies often rely on the Atomic Force Microscope (AFM), which allows investigating the physical properties at the nanoscale of materials [3, 4] and of biomolecules [5, 6]. In this contribution, we will show how the set of these microscopes (SEM, FIB, AFM) can be smartly used to investigate fundamental aspects in Biology, Materials Science and Nanomagnetism. In particular, we will show examples where the SEM and FIB microscopes are used in combination with a precursor gas to grow nanotips at the apex of an AFM, techniques known as Focused Electron Beam Induced Deposition (FEBID) and Focused Ion Beam Induced Deposition (FIBID). These nanotips are subsequently applied to the investigation of the functional properties of magnetic thin films, nanopatterned structures, proteins and DNA.

[1] Nanofabrication, J. M. De Teresa (Ed.), IOP (U.K.) 2020, doi: 10.1088/978-0-7503-2608-7
[2] Höflich K. et al., Appl. Phys. Rev. 2023, 10, 041311
[3] Escalante-Quiceno T. et al., Low Temp. Phys. 2024, 50, 825
[4] Escalante-Quiceno T. et al., Sensors 2023, 23, 2879
[5] Allen F., De Teresa J. M., and Onoa B., ACS Appl. Mater. & Inter. 2024, 16, 4439
[6] Marcuello C. et al., manuscript under preparation

204	**Direct-Write Fabrication of Silver Nanostructures with Metallic behaviour and High-Performance SERS Response via FIB Irradiation of Organometallic Films**	Juan Ignacio Ocaña Parral	Contributed talk (11:45-12:00)

Juan Ignacio Ocaña Parral (1) Sven Barth (2) Pilar Cea (3) Jose Maria de Teresa (1) Lucía Herrer (1) Alba Salvador-Porroche (1) Soraya Sangiao (1,4) Inés Tejedor (1)

(1) Instituto de Nanociencia y Materiales de Aragón (CSIC-Universidad de Zaragoza)
(2) Goethe-University Frankfurt
(3) University of Zaragoza
(4) Laboratorio de Microscopías Avanzadas, Universidad de Zaragoza

Metallic nanopatterns exhibit unique electrical and optical properties, making them highly attractive for applications in nanoelectronics, nanophotonics, and sensing technologies. However, conventional fabrication techniques often face trade-offs between resolution, throughput, and cost-effectiveness, motivating alternative approaches [1]. Here, we present a versatile, resist-free method for fabricating silver micro- and nanostructures via direct decomposition of spin-coated silver butyrate films by Focused Ion Beam (FIB) irradiation. The process combines (i) spin coating, (ii) focused Ga^+ irradiation, and (iii) development by removing non-irradiated material. By tuning precursor composition and irradiation conditions, we achieve precise control over the microstructure, from continuous Ag-enriched platelets to nanoparticle assemblies. This enables dual functionality: continuous structures show metallic

behaviour with resistivity as low as 90 μΩ·cm, while nanoparticle-based morphologies act as efficient Surface-Enhanced Raman Spectroscopy (SERS) substrates, with enhancement factors comparable to state-of-the-art commercial silver substrates.
Overall, this approach provides a simple and flexible route to engineer silver nanostructures with tailored electrical and plasmonic properties, opening opportunities in nanoelectronic interconnects and SERS-based sensing.

[1] Alongkorn Pimpin et al. Engineering journal. 2012, 16, pp. 37–56.

488	**Development of heavy noble gas field ion sources using an iridium coated single crystalline tungsten emitter**	Amina Zid	Contributed talk (12:00-12:15)

Amina Zid (1) Anne Delobbe G. Hlawacek (1) Arnaud Houel (1) Nico Klingner (1)

(1) Ion Beam Center, Helmholz-Zentrum Dresden-Rossendorf, Dresden, Germany

Gas Field Ion Sources (GFIS) have already demonstrated their efficiency in nano imaging and patterning due to their high brightness, high current density and superior spatial resolution [1]. This type of ion source typically employs light noble gases such as helium and neon. In the first case, negligible sputtering and fast diffusion enables image resolution as low as 0.5nm, while the latter allows high resolution milling of small nanostructures with resolutions milling of small nanostructures with resolutions better than conventional Liquid Metal Ion Source (LMIS). GFIS suffers from limitation in terms of material removal rate due to low current. Another limitation comes from the light ion species used, as well as bubble formation due to deep implantation making GFIS less efficient than LMIS for larger volume or high aspect ratio milling application with only shallow end of range defects. To overcome those limitations, we investigated GFIS performance in a Focused Ion Beam (FIB) using heavier noble gases, namely argon and xenon.
In addition, we consider an alternative emitter configuration. Historically, GFIS emitters are based on single-crystal tungsten tips while, we employed an iridium coated tungsten tip. Among noble metals, iridium confers the strongest bond with tungsten [2]. That particularity would allow the overall tip structure to withstand higher electric field than with any other noble metal coating. As a result, iridium coated tip enable higher beam currents without endangering the emitter stability. We also work with a single emission point opposed to the typically trimer configuration traditionally used in Helium Ion Microscope (HIM).
In this work we will present the first FIB evaluation and performances of this particular emitter using argon and xenon. Comparison to helium and neon based GFIS used in the HIM will also be covered.

[1] Höflich, K.; et al. Roadmap for focused ion beam technologies. Applied Physics Reviews 2023
[2] Oshima, C.; Tomitori, M.; Shimoda, T.; Yasaka, A.; Asai, H.; Rokuta, E. Thermal Stability of Single-Atom Termination at a Pyramidal Apex of an Ir-W Tip. Surface Science and Nanotechnology 2018

784	**Computational multiscale modelling of the nanopillar growth using focused electron beam induced deposition**	Alexey Verkhovtsev	Contributed talk (12:15-12:30)

Alexey Verkhovtsev (1) Gennady Sushko (1) Jorim Kornblueh (2) Ilia A. Solov'yov (2) Andrey V. Solov'yov (2)

(1) MBN Research Center, Altenhöferallee 3, 60438 Frankfurt am Main, Germany
(2) Institute of Physics, Carl von Ossietzky University Oldenburg, Carl-von-Ossietzky-Str. 9-11, 26111 Oldenburg, Germany

This talk will present the key elements of the computational multiscale modelling approach to simulating 3D nanofabrication using focused electron beam-induced deposition (FEBID) [1-5]. This approach is based on computational algorithms (Irradiation-Driven Molecular Dynamics [2] and Stochastic Dynamics – SD [5,6]) implemented in the advanced software package MBN Explorer [7], which is being developed by the MBN Research Center in Frankfurt (https://www.mbnresearch.com/).
The talk will focus specifically on our recent SD simulation results for nanopillar growth using FEBID [5,8]. The SD method uses probabilistic theory to describe the FEBID process, involving particles that represent intact precursor molecules, their fragments, ligands, and the substrate [5,7]. This modelling approach incorporates a detailed description of elementary processes, including precursor adsorption, diffusion, desorption, dissociation, and the growth of metal-containing deposits. As an illustrative case study, we have analysed the growth of nanopillars using the FEBID of W(CO) precursors on a SiO substrate under 30 keV electron beam irradiation. The simulation protocol accounts for realistic irradiation/replenishment cycles, precursor injection flux, and fragmentation rates, which are derived from track-structure Monte Carlo simulations [5].
The simulation results are systematically validated against relevant experimental data [9] in terms of deposit's composition, size and growth rate. Importantly, the simulations provide a detailed characterisation of the deposit's structure at a nanoscopic level. The utilized multiscale modelling approach provides a robust foundation for predictive simulations of irradiation-driven fabrication processes and their applications in FEBID-based 3D-nanoprinting.
The authors acknowledge the support received through the COST Innovators Grant project IG20129 INDICO, which is supported by COST (European Cooperation in Science and Technology).

[1] A.V. Solov'yov et al., Chem. Rev. 124 (2024) 8014-8129
[2] G.B. Sushko, I.A. Solov'yov, A.V. Solov'yov, Eur. Phys. J. D 70 (2016) 217
[3] P. de Vera, M. Azzolini, G.B. Sushko, I. Abril, I., R. Garcia-Molina, M. Dapor, I.A. Solov'yov, A.V. Solov'yov, Sci. Rep. 10 (2020) 20827
[4] A. Prosvetov, A.V. Verkhovtsev, G. Sushko, A.V. Solov'yov, Phys. Chem. Chem. Phys. 24 (2022) 10807
[5] I.A. Solov'yov, A. Prosvetov, G. Sushko, A.V. Solov'yov, https://arxiv.org/abs/2506.18163 (2025)
[6] I.A. Solov'yov, G. Sushko, I. Friis, A.V. Solov'yov, J. Comput. Chem. 43 (2022) 1442
[7] I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, and A.V. Solov'yov, J. Comput. Chem. 33 (2012) 2412
[8] A.V. Verkhovtsev, G. Sushko, J. Kornblueh, I.A. Solov'yov, A.V. Solov'yov (in preparation, 2026)
[9] J.D. Fowlkes, P.D. Rack, ACS Nano 4 (2010) 1619

M30 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
705 **P066**	**W-C Nanocomposites via Xe? Plasma Focused Ion Beam Induced Deposition**	Jan Michalik	Poster

Jan Michalik (1) Aleksandra Szkudlarek (2) Krzysztof Maćkosz (3)

(1) AGH University of Krakow; Faculty of Physics and Applied Computer Science
(2) AGH University of Krakow, Academic Centre for Materials and Nanotechnology
(3) Mechanics of Materials and Nanostructures, Empa-Swiss Federal Laboratories for Materials Science and Technology

Focused Ion Beam Induced Deposition (FIBID) provides a versatile route for nanoscale fabrication, though the resulting material properties are highly sensitive to ion species and processing parameters. Our present study investigates the Xe^+-ion-assisted deposition of W-C composites using a tungsten carbonyl precursor. The effects of beam energy and current on the composition, surface morphology, and microstructure were systematically characterized using SEM/EDX, AFM, and TEM.
For comparison, Ga^+-induced deposits were fabricated under comparable conditions to isolate the influence of the ion species on precursor dissociation and impurity levels. Results demonstrate that Xe-FIBID produces denser nanocomposites with significantly reduced contamination compared to Ga^+-based methods. These findings offer critical insights into ion-matter interactions and position Xe plasma FIB systems as superior tools for high-purity nanofabrication and device prototyping.

152 **P067**	**Direct-Write Fabrication of Ultrathin Nb–Based Memristive Devices by Focused Electron Beam Induced Deposition**	Harald Plank	Poster

Sabrina Menhart (1) Sven Barth (2) Harald Plank (1)

(1) Graz University of Technology
(2) Goethe-University Frankfurt

Over the past decade, additive direct-write nanomanufacturing has emerged as a powerful approach for the localized synthesis of functional materials with minimal constraints on substrate choice or geometry. Among the available nanoscale techniques, Focused Electron Beam Induced Deposition (FEBID) has gained increasing attention due to its capability to directly synthesize nanostructures from precursor molecules with nanometer-scale precision. While FEBID is now widely recognized for the fabrication of complex 3D architectures, its potential for the direct synthesis of functional electronic materials in planar device geometries remains relatively unexplored. In particular, beam-written materials for memristive devices represent a promising route toward highly localized neuromorphic hardware elements and may ultimately enable adaptive networks extending even into three dimensions.
Here, we investigate the feasibility of synthesizing Nb-based memristive materials using FEBID from a Nb(NMe)(N-t-Bu) precursor. First, we confirm that the precursor enables reliable deposition of Nb-containing structures. A systematic parameter study is then performed to identify process windows allowing the fabrication of sub-nanometer-flat, homogeneous deposits, which are essential for integration in memristive devices. The intrinsic electrical properties of the resulting Nb–N–O material are subsequently evaluated using multi-electrode test structures. In this context, the influence of post-growth treatments, including electron beam curing, H_2O-assisted purification, and ambient exposure, is examined. It is found that the electrical behavior remains largely stable across these processing conditions, indicating robust conduction pathways within the material.
Based on these findings, stacked Au–(Nb–N–O)–Co_3Fe devices are fabricated with progressively reduced active layer thicknesses. While intermediate thicknesses (≈ 50–15 nm) exhibit stable conduction behavior with only minor processing dependencies, clear memristive characteristics emerge when the active layer thickness is reduced to the sub-5 nm regime. In such geometries, the devices show reproducible hysteretic I–V behavior following a short conditioning phase during the first measurement cycles. In contrast to purely ohmic conduction, a non-linear transport characteristic is observed. This suggests field-assisted conduction through defect states within the ultrathin Nb–N–O layer, consistent with trap-mediated transport mechanisms. Within this picture, charge transport is governed by the filling and emptying of localized defect states, giving rise to non-linear current–voltage behavior and the formation of dynamically evolving conductive pathways across the ultrathin layer, as commonly observed in amorphous nanogranular materials.
These results demonstrate that FEBID enables the direct synthesis of Nb-based memristive materials and provides a promising starting point for further research towards nanoscale memristive devices and beam-written neuromorphic architectures, both in planar and future 3D device designs.

153 **P068**	**Magnetic-Conductive MC Nanoprobes for Advanced AFM Fusing Functionalities via 3D Nanoprinting**	Harald Plank	Poster

Lukas Seewald (1) Michele Brugger-Hatzl (2) Robert Winkler (1) Sven Barth (3) Harald Plank (1)

(1) Graz University of Technology
(2) Graz Centre of Electron Microscopy
(3) Goethe-University Frankfurt

Atomic Force Microscopy (AFM) has emerged as an indispensable research and development tool for imaging and analyses down to the lowest nanoscale. Employing a sharp probe affixed to a cantilever, AFM achieves (sub-)nanometer resolution by raster scanning across a sample surface, effectively circumvent-ing Abbe's limit. This remarkable capability extends to various atmospheres, vacuum and even liquid environments, making AFM extremely flexible in application. Advanced operation modes and functional-ized probes enable comprehensive investigations beyond surface topography, encompassing electrical, mechanical, optical, mechanical, thermal, and magnetic properties. However, traditional probe function-alization methods involving coatings often compromise resolution due to increased apex radii and pose the risk of delamination, potentially rendering the probe ineffective or entirely useless. An innovative approach to creating functional probes circumvents these limitations through Focused Electron Beam Induced Deposition (FEBID)-based 3D nanoprinting, as demonstrated for thermal, optical, electrical and magnetic properties.
Here, we demonstrate the first FUSION-probe concept, which combines magnetic (MFM) and electrical capabilities (CAFM), termed MC Fusion Probe. We hereby aim at improving correlative microscopy by eliminating the need to change between different probes, not only to safe time but, more importantly, to eliminated the time consuming and often challenging rediscover of highly localized regions of interest even without fiducials. The main hurdle of this integration process is the fact, that CAFM is performed in contact mode employing a soft cantilever, while MFM uses an oscillating cantilever intermittently tapping the sample surface which requires a stiffer cantilever for stable operation. This in turn increases contact forces in contact mode, raising mechanical demands of the probe. Our probe concept is fabricated via FEBID from a CoFe precursor, yielding a highly crystalline microstructure with minor C and O residues. These probes have recently demonstrated superior and long-lasting MFM performance, and due to their purity should be conductive as well. As a first step, wear tests were carried out to confine the range of cantilever spring constants for reliable operation in both AFM modes. Subsequently, the probe

concept was adapted to self-sensing cantilever systems enabling application in Quantum Design Microscopy's FUSIONScope™, a deeply integrated SEM-AFM system. In combination with the already patented Simulta-neous Measurement Operation (SMO) ideal surroundings are established to operate the MC Probe to its full potential, seamlessly adding measurement capabilities without the need to switch between probes, which is illustrated on different samples. Thus, we unveil a sophisticated FEBID-based, multi-functional probe concept, poised to elevate correlative microscopy to new heights, with additional groundbreaking concepts on the future horizon.

154 P069	**Functional Imprinting: Local Modification of Beam Induced Deposits**	Harald Plank	Poster

Anna Weitzer (1) David Loibner (1) Verena Reisecker (1) Lukas Seewald (1) Robert Winkler (1) Harald Plank (1)

(1) Graz University of Technology

Additive manufacturing of nanoscale structures on a myriad of substrate types and surface morphologies stands as a prominent distinguishing feature of Focused Electron Beam Induced Deposition (FEBID) and Focused Ion Beam Induced Deposition (FIBID). Beyond the mere creation of bulky, planar, and simplistic pillar geometries, the controlled fabrication of intricate 3D nano-architectures has catalyzed a revolution in this realm of nanofabrication. That stems from its unparalleled prowess in design complexity, predicta-bility, reliability, feature sizes, and functional variability, which strongly improved over the last decade. However, the aspect of functionality often grapples with challenges posed by incomplete precursor dis-sociation, resulting in infamously high carbon contents that can diminish or entirely mask the intended functionalities upon initial fabrication. To leverage material quality and precisely tailor them to applica-tion requirements, post-processing techniques such as thermal treatments, exposure to gases, and/or irradiation with photons/electrons/ions prove indispensable as successfully demonstrated by many dif-ferent studies. While conventionally applied to the entire FEBID object in the past, we now embark on the next logical progression by introducing a paradigm shift: selective area modification, dubbed as func-tional imprinting. This innovative approach allows for the integration of functional regions boasting di-verse designs within the surrounding pristine material, thereby serving as a scaffold with varied proper-ties tailored for distinct purposes, e.g. embedding of plasmonically active elements in a flexible design.
In this contribution, we delve into two innovative post-processing methodologies, both harnessing the implications of a focused electron beam together with its complex behavior in solid materials for dynamic shape imprinting. Both concepts, however, use the local instead of a global application to the deposit of interest, which opens up new possibilities. The first concept, electron beam curing (EBC), involves sub-jecting deposits to an electron beam within vacuum conditions with no precursor gas present. This tech-nique offers a spectrum of possibilities, ranging from inducing statistical grain growth for electric conduc-tivity refinement, to manipulating the carbonaceous matrix with mechanical implications, and even achieving asymmetric stress-strain for the controlled bending of 3D objects, surpassing conventional fabrication constraints. As for the second approach, electron exposure in low-pressure, room tempera-ture water vapor serves to eliminate residual carbon from original deposits. Here, we meticulously assess this methodology by orchestrating local material transfer from pristine AuC composition into pure gold, meticulously exploring design potentials, intrinsic limitations, and functional attributes of the transformed areas. The latter shows plasmonic activities with high lateral resolution as discussed in this contribution. Through these endeavors, we establish the groundwork for advanced local material tuning of FEBID/FIBID materials, potentially heralding novel application vistas at the nanoscale.

171 P070	**Optimization of Horizontal Nanowire Growth in FEBID for 3D Nanoprinting**	Gabriel Andrade de Paula	Poster

Gabriel Andrade de Paula (1) Le Zhao (1) Jakub Mateusz Jurczyk (1) Amalio Fernandez-Pacheco (1)

(1) TU Wien

The controlled fabrication of horizontal nanowires with multiple contact points to a substrate is significant for applications in nanoelectronics, circuit design, and advanced characterization techniques. Such geometries enable well-defined electrical interfacing and increased flexibility in device integration. However, their realization via additive nanofabrication remains challenging. In particular, focused electron beam induced deposition (FEBID), despite its versatility for direct-write 3D nanostructuring, intrinsically favours vertical growth due to localized precursor dissociation and electron–matter interactions [1,2]. In this work, we investigate the optimization of horizontal nanowire growth using FEBID in combination with the layer-by-layer 3D nanoprinting software f3ast. Key beam parameters, including electron beam current and acceleration voltage, are systematically varied together with the stage angle, while the dwell times and growth rate are defined within the f3ast patterning routine. The results demonstrate that controlled modulation of these parameters enables the fabrication of stable nanowires with controlled geometry, allowing for the formation of straight segments. Lower acceleration voltages combined with optimized beam currents are found to enhance lateral growth by promoting surface-confined energy deposition. These findings help establish practical guidelines for the reliable fabrication of simple and complex horizontal architectures which can be used in 3D spintronics.

[1] L. Skoric, et al. Layer-by-Layer Growth of Complex-Shaped Three-Dimensional Nanostructures with Focused Electron Beams, Nano Letters (2020) 20 (1), 184-191
[2] R. Winkler, et al. High-Fidelity 3D-Nanoprinting via Focused Electron Beams: Growth Fundamentals, ACS Applied Nano Materials 2018 1 (3), 1014-1027

323 P071	**Python-Based Automation of 3D FEBID Nanofabrication**	Stefan Mikulik	Poster

Stefan Mikulik (1) Jakub Mateusz Jurczyk (1) Amalio Fernandez-Pacheco (1)

(1) TU Wien

The reliable fabrication of complex three-dimensional nanostructures via focused electron beam induced deposition (FEBID) requires precise control over a wide range of process parameters [1]. Conventional workflows rely heavily on manual operation, limiting reproducibility, throughput, and scalability. Automation is therefore the key to faster prototyping and application-oriented nanofabrication.
In this work, we present a Python-based automation approach that integrates the layer-by-layer 3D nanoprinting software f3ast into the patterning control of a scanning electron microscope (SEM) [2]. The system interfaces with key instrument components, allowing for stage motion, gas injection system (GIS) operations, and electron optics adjustments, enabling fully automated deposition sequences. A central element is a robust autofocus routine tailored for FEBID. To this end, we investigated gradient- and variance-based focus metrics, combined with algorithmic region-of-interest selection and noise reduction, and evaluated the reproducibility of the resulting focus under varying deposition conditions and sample geometries [3]. The routine is embedded into the deposition workflow and executed at predefined positions prior to each writing step to ensure consistent beam focus and placement. Its performance is evaluated using standard calibration patterns for f3ast, enabling quantitative assessment of focus quality based on these well-understood structures.
In addition, we implement a feedback loop that evaluates deposited calibration structures and estimates f3ast calibration parameters, enabling adaptive optimization of the fabrication process. Together, the integration of automated focusing, deposition, and feedback-driven parameter adjustment enables

reproducible FEBID processes, while reducing operator workload and supporting efficient, high-throughput nanoscale prototyping with minimal user intervention.

[1] V. Reisecker, R. Winkler, H. Plank, Adv. Funct. Mater. (2024). https://doi.org/10.1002/adfm.202407567
[2] L. Skoric et al., Nano Lett. (2019). https://doi.org/10.1021/acs.nanolett.9b03565
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84 **P072**	**Cryogenic Focused Ion Beam for the study of anisotropy in the magnetotransport properties of bismuth**	Amaia Sáenz-Hernández	Poster

Amaia Sáenz-Hernández (1) Soraya Sangiao (1,2) Claudia Felser (3) Chandra Shekhar (3) José Ángel Pardo (1,2) Alfonso Ibarra (2) Ángel Larrea (1) Jose Maria de Teresa (1)

(1) Instituto de Nanociencia y Materiales de Aragón (INMA), CSIC-Universidad de Zaragoza
(2) Laboratorio de Microscopías Avanzadas, Universidad de Zaragoza
(3) Max-Planck-Institute for Chemical Physics of Solids

The study of anisotropic magnetotransport in quantum materials is of significant interest, although sample preparation remains challenging[1]. Focused ion beam (FIB) has become one of the most widely used techniques for microcrystal device fabrication, however, it is typically combined with other techniques, frequently involving the use of chemical resists[2].
Our research group has developed an in situ fabrication method using FIB exclusively, allowing the study of anisotropic magnetotransport in microscale single crystals that cannot be synthesized into thin films. Two types of devices are fabricated: Horizontal (H), where current flows perpendicular to both the crystallographic c-axis and magnetic field, and Vertical (V), with current parallel to the c-axis and perpendicular to the field (see Figure)[3].
We present magnetotransport measurements on single-crystal bismuth microdevices of both types. As Bi is observed to melt under Ga^+ FIB irradiation at room temperature, two low-temperature fabrication approaches are implemented: an N_2-based cryo module and a Peltier stage. Devices show the very large magnetoresistance expected from bismuth as well as clear differences in the Shubnikov–de Haas oscillations of the V and H samples[4].

[1] M. Ziese, et al., J. Condens. Matter Phys. 2000, 12, 13.
[2] P.J.W. Moll, et al., Condens. Matter Phys. 2018, 9, 147–162.
[3] A. Saenz-Hernandez, et al., MRS Commun. 2025, 15, 414
[4] A.Sáenz-Hernández, et al., Adv. Funct. Mater.. 2026, 20, e17475.

566 **P073**	The fate of organic ligands in gas assisted e-nanoprinting of metals	Ivo Utke	Poster

Ivo Utke (1) Jakub Mateusz Jurczyk (2) Amalio Fernandez-Pacheco (2)

(1) EMPA
(2) TU Wien

Amongst the various 3D metal additive manufacturing methods that have been recently reviewed [1], nanoprinting with focused electron beams offers the greatest shape flexibility and the smallest print size. The technology is rooted in the high-tech industry as a powerful maskless, minimally invasive nanofabrication platform for mask repair, cantilever probe functionalization, and biosensors.
A persisting challenge is the limited number of pure materials that can be reproducibly e-beam nanoprinted when typical volatile metalorganic molecules are involved. The removal of the organic ligands from the metal atom and the surface is governed by a delicate interplay of both surface mediated thermal and electron induced non-thermal mechanisms involved in this approach [2]. To achieve high metal content nanoprinting, for now, the paradigm is to use small ligands in metalorganic molecules. This may serve (i) reducing potential e-fragmentation of large ligands containing several atoms and bonds into non-volatile co-deposited fragments and (ii) enhance desorption of the ligands dissociated from the parent molecule. Recently, however, large ketoesterate ligands in Pd(tbaoac)2 and Cu(tbaoac)2 precusors were also shown to be removed by up to 90% of their initial presence in the molecule [3, 4].
Here we present our recent continuum modeling activities to rationalize the metal content to be expected in e-nanoprinted structures [5]. We consider the complete removal of ligands in terms of their mean surface residence time and their further fragmentation into non-volatile moieties by electrons. Solving the system of coupled differential equations defines the electron exposure parameters needed to perform e-nanoprinting within the ligand-desorption-driven regime for highest metal content. We conclude with a comparison to experiments.

[1] A. Reiser et al., Adv. Funct. Mater. 2020, 1910491, DOI: 10.1002/adfm.201910491.
[2] I. Utke, P. Swiderek, K. Höflich, K. Madajska, J. Jurczyk, P. Martinovic, I.B. Szymanska, Coord. Chem. Reviews 445 (2021), 213851, https://doi.org/10.1016/j.ccr.2021.213851.
[3] C. Haverkamp, G. Sarau, M.N. Polyakov, I. Utke, M.V. Puydinger Dos Santos, S. Christiansen, K. Höflich, Beilstein J. Nanotechnol. 2018, 9, 1220–1227, doi:10.3762/bjnano.9.113.
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[5] J. Jurczyk, L. Brockhuis, A. Fernández-Pacheco, I. Utke, Small Methods 2025, e01956, https://doi.org/10.1002/smtd.202501956

M31 - Metal and Metal Oxide Particles for Catalysis and Sensorics

M31 – Session 1 (Thu 24, 10:30-12:30, Chair: Wolfgang Ernst)			
ID	Title	Speaker	Type
267	**Structure and Dynamics of Metal Clusters**	Rolf Schäfer	Invited talk (10:30-11:00)

Rolf Schäfer (1)

(1) TU Darmstadt

Metal clusters consisting of about a dozen atoms exhibit many properties different from those of the corresponding bulk material, which is due to the strong influence of the particle surface as well as to quantum size effects. It is therefore of great interest to study the evolution of their geometric and electronic structure as a function of size. The presentation introduces our approaches for investigating isolated clusters in the gas phase and clusters supported on surfaces. This includes the study of the dielectric, optical, magnetic and catalytic properties of mass-selected clusters. The main goal is to uncover correlations in the geometric and electronic structure and thus contribute to a better understanding of the magnetic and catalytic behavior of nanoclusters as a function of size and chemical composition.

351	**Cluster beam deposition of bimetallic nanoalloys: From gas-phase growth to catalytic function**	Ewald Janssens	Invited talk (11:00-11:30)

Ewald Janssens (1)

(1) KU Leuven

Beam deposition of mass-selected bimetallic clusters produced in a laser ablation source provides a powerful platform to investigate cluster–surface interactions and to establish structure–activity relationships in well-defined catalytic systems. The combination of controlled gas-phase growth, soft landing, and detailed post-deposition characterization enables systematic studies of structural, chemical, and electronic properties of supported nanoalloys before, during, and after reaction.
Deposition of gas-phase produced Au_xCu_{1-x} clusters (x = 1, 0.75, 0.5, 0.25 and 0) onto TiO_2 nanotubes was found to significantly enhance photoelectrochemical water splitting. Detailed structural and chemical analysis reveals segregation-driven formation of bifunctional catalytic sites composed of metallic Au/AuCu domains in contact with a copper oxide surface layer. These findings highlight how cluster composition and restructuring upon deposition determine interfacial properties and catalytic performance [1].
To bridge cluster-based model studies and realistic catalytic environments, a dedicated microreactor was developed to probe minute quantities of beam-deposited nanoparticles under elevated pressures (up to 40 bar) and temperatures (up to 250 °C). $PdZnO_x$ and $CuZnO_x$ clusters soft-landed on oxide and carbon supports were investigated for CO_2 hydrogenation via the reverse water–gas shift reaction [2] and methanol synthesis [3]. By tuning alloying and oxidation during cluster growth through the aggregation atmosphere, catalytic activity and selectivity could be controlled.
These results demonstrate how cluster beam deposition links gas-phase nanoalloy formation with surface-supported functionality, providing insight into alloying, segregation, metal–support interactions, and their impact on catalytic performance.

[1] V.C. Chinnabathini, K.R. Ag, T.H.T. Nguyen, Z. Zarkua, I. Abbas, T.H. Hoang, P. Lievens, D. Grandjean, S.W. Verbruggen, E. Janssens, Nanoscale 17, 833 (2025).
[2] I. Abbas, F. Romeggio, K. Pilarczyk, S. Kuhn, C.D. Damsgaard, J. Kibsgaard, P. Lievensa, D. Grandjean, E. Janssens, Chem. Eng. J. 503, 158127 (2025).
[3] I. Abbas, W. Ji, et al., in preparation (2026)

443	**Charge and electronics in dinitrogen activation by transition metal clusters**	Gereon Niedner-Schatteburg	Contributed talk (11:30-11:45)

Gereon Niedner-Schatteburg (1)

(1) RPTU Kaiserslautern-Landau

Isolated gas phase clusters of atoms and molecules serve as well established proxys for the characterization of elementary steps and intermediates within complex reactions at ambient or industrial conditions. In this context, the charge states of such clusters are subject of debate ever since. We have developed and applied a cryo trapping technique [1] that allowed us to characterize size selected transition metal clusters and their adsorbates for their kinetic and spectroscopic properties, and we have applied this technique to clusters of several transition metals and some of their alloys [2-8]. Electronic characterization arose through novel X-ray techniques which we have brought to application at our gas phase clusters [9]. On the basis of our wide spread results from these experiments we have recently started a systematic quantum chemical survey of charge states and shifts along the N2 activating reaction pathways of some selected clusters [10], and the conceptual findings of this survey shall be presented, and their implications and the outreach shall be discussed.

[1] DOI: 10.1016/B978-0-12-814013-0.00019-3; [3] DOI: 10.1039/c5cp00047e; [2] DOI: 10.1021/acs.jpcc.6b12167; 10.1063/1.4997403 ; 10.1063/1.4997407; [5] DOI: 10.1007/s11244-017-0865-2 ; 10.1080/00268976.2021.1953172; [4] DOI: 10.1063/5.0064965 ; 10.1063/5.0064966; [5] DOI: 10.1063/5.0075289 ; 10.1063/5.0075286; [7] DOI: 10.1039/D0CP06208A ; 10.1063/5.0157218 ; 10.1063/5.0157217; [8] DOI: 10.1021/acs.jpclett.8b00093 ; submitted to Helv. Chim. Act.; [9] DOI: 10.1103/PhysRevLett.107.233401 ; 10.1039/C5CP01923K ; 10.1063/1.4929482; [10] to be published

730	**Multiple roles of metal nanoparticles in tuning surface reactivity**	Alexander Genest	Contributed talk (11:45-12.00)

Alexander Genest (1)

(1) Institute of Materials Chemistry, TU Wien

Metal nanoparticles offer a variety of largely independent handles for tailoring catalytic performance - size, shape, and their interaction with the support. DFT calculations, mostly carried out with VASP, allow us to explore this design space, to connect macroscopic activity as well as selectivity trends to specific surface motifs at the atomic scale.

Using CO as probe molecule at Pd, the adsorption energy is determined to depend systematically on the geometry of the local site, with the metal-metal bond lengths at the adsorption site serving as descriptor [1]. Extending this site-resolved picture over particle sizes from 13 to ~150 atoms yields a non-monotonic scaling behavior. A steep drop from very small clusters meets a slow decrease from the asymptotic bulk-surface value, leaving an intermediate-size regime with the weakest CO binding at the intersection of the two competing trends [2]. Particle size thus acts as a first control for adsorption strength.
A second, more subtle role emerges in 1-butene hydrogenation and isomerization on Pd/Al_2O_3 [3]. Selectivity here is not governed by an electronic modification of individual atoms, but by the change in abundance of (111), (100) and edge sites as the particle size varies - a structural effect rationalized by combining DFT with microkinetic modeling.
A third role is played by the support. On graphite-supported Ag, Au and Cu nanoparticles, the carbon is far from innocent. At the metal–carbon three-phase boundary the availability of hydrogen is strongly enhanced, raising the per-atom activity in ethylene hydrogenation by up to two orders of magnitude [4].
Given this many independent levers at hand, the broad deployment of metal nanoparticles in heterogeneous catalysis is hardly a coincidence.

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[3] A. Genest, J. Silvestre-Albero, W.-Q. Li, N. Rösch, G. Rupprechter, Nat. Commun. 12 (2021) 6098.
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M31 – Session 2 (Thu 24, 16:00-18:00, Chair: Günther Rupprechter)

ID	Title	Speaker	Type
463	**The Power of Imperfections: A New Paradigm in Catalysis**	Beatriz Roldan Cuenya	Invited talk (16:00-16:30)

Beatriz Roldan Cuenya (1)

(1) Fritz-Haber-Institut der Max-Planck-Gesellschaft

The recycling of waste products from human activities is a cornerstone of sustainable production and energy systems. In this context, the electrochemical production of basic chemical feedstocks such as hydrogen, ethanol or ammonia using green electricity plays a key role. To make such processes more active, selective and scalable, we need better catalysts than those available today. The latter requires fundamental understanding of the dynamic structure of the catalytic materials while they are performing their function, i.e. “operando”.
My talk will illustrate that morphologically and chemically well-defined pre-catalysts experience drastic modifications under operation, and that such evolving nanoscale surface structure governs the selectivity and kinetics of the reactions. Examples will be drawn from the study of the electrochemical CO_2 reduction (CO_2RR), nitrate reduction to ammonia, and the oxygen evolution reaction (OER). The model pre-catalysts studied here will range from size and shape-controlled nanoparticles (Cu_2O cubes and octahedra, CoOx NPs, $Ni(OH)_2$, $Co(OH)_2$ and Co_2FeO_4 nanoplatelets) to epitaxial thin films (Co_3O_4, $Co_{1+\delta}Fe_{2-\delta}O_4$, NiO). The need of a synergistic multi-technique operando microscopy (EC-TEM, EC-AFM, LEEM), spectroscopy (XAS, Raman, XPEEM) and diffraction (HE-SXRD) approach will be evidenced in order to follow the active state formation, its deactivation, or regeneration pathways. Correlations between the dynamic structure and composition of the catalysts and their activity, selectivity and durability will be featured. Moreover, special attention will be given to unveiling the role of impurities (Fe) on the catalyst activation in OER, as well as of electrolyte cations (K, Na, Li, Cs) in the kinetics of the formation of different active “frustrated” oxy-hydroxide phases during OER or in the catalyst surface restructuring during CO_2RR.

ID	Title	Speaker	Type
562	**Metal Nanoparticle Catalysts for Hydrogen Evolution**	Alessandro Fortunelli	Invited talk (16:30-17:00)

Alessandro Fortunelli (1) Olanyian Okikiola (1) Thantip Roongcharoen (1)

(1) Italian National Research Council (CNR)

I will focus on the reaction of Hydrogen Evolution, i.e., the catalytic process by which H2 gas is evolved from a system, a process of interest in both electrochemical and thermal catalytic contexts.
As an example of an electrochemical process, I will present recent results on the use of a FeCoNiAlSi High-Entropy Alloy as a Hydrogen Evolution Reaction (HER) catalyst (a material previously proposed as a potentially very efficient ammonia synthesis catalyst), and I will show how this material possesses favorable features also as an electrochemical HER catalyst. From the analysis of the results, I will then try to single out those features that make a material a potential candidate for the HER process.
As an example of a thermal process, I will present recent results on platinum-based systems, in particular extended platinum facets either bare or covered with a ultrathin TiOx (TiO2 defective) phase. I will show that such oxide overlayers do slow down the hydrogen evolution ability of platinum, but, under given conditions, not at the point of suppressing it, thus offering an example of a reasonable compromise between catalytic activity and environmental stability. If time will allow, I will conclude with an example of an inner-oxide core-shell HER catalyst material.

ID	Title	Speaker	Type
719	**Redox dynamics of Co and Cu nanotips imaged by in situ field emission microscopy**	Johannes Zeininger	Contributed talk (17:00-17:15)

Johannes Zeininger (1) Alexander Blocher (1) Günther Rupprechter (1)

(1) Institute of Materials Chemistry, TU Wien, Vienna, Austria

Metal nanoparticles in reactive atmospheres are not static. Redox cycling reshapes their surface and generates transient oxide species, affecting catalytic performance. Field emission microscopy (FEM) is applied to Co and Cu nanotips to follow this interplay at nm and ms resolution which enables feature-resolved observation of oxidation and reduction during hydrogen oxidation at 10^{-5} mbar.
On the annealed Co tip, oscillations were resolved, with an FEM signature of periodic splitting of single bright spots into symmetric triplets. We relate this nano-scale feedback process to the growth and collapse of (111)-truncated edges of Co cubes. Ex-situ scanning electron microscopy (SEM) confirmed that the Co apex had transformed into cubic oxide grains. In previous environmental SEM measurements of the same system dynamics, oxide related volume increase initiated porous networks and regulated pore diameter. However, the mechanistic origin of dynamics expected within pores could not be investigated. Correlating in-situ/operando microscopy insights by shared metrics of dynamic behavior allows to bridge mechanistic understanding over

length scales. On Cu tips, for similar experiments, a complex self-organization was resolved. Spatiotemporal analysis identified classes of pattern dynamics and their interplay, including periodic explosion-like events ending bright spots that occurred at high field strengths. Ex-situ SEM imaged a canyon-and-plateau topography consistent with combined oxide growth and H-assisted field evaporation of its sharp edges.
Overall, we demonstrate how cyclic redox dynamics transiently modifies nanoparticle morphologies and local reaction. In this way, employing self-sustained oscillations as a probe, controlled oxidation and reduction processes are accessed at the nanoscale with high temporal resolution within a single experiment.

465	**Advanced Electron Microscopy of Metal Clusters Grown Inside Superfluid Helium Droplets**	Ferdinand Hofer	Contributed talk (17:15-17:30)

Wolfgang E. Ernst (1) Ferdinand Hofer (1) Daniel Knez (1) Gerald Kothleitner (1)

(1) Graz University of Technology

Through aggregation inside superfluid helium droplets, metal nanoparticles and core-shell clusters of different morphology are generated and deposited on solid carbon, h-BN, ITO, or SiN substrates. The created nanoparticles are characterized by temperature dependent electron microscopy, up to 1000 degrees C, energy-dispersive x-ray spectroscopy, electron energy loss spectroscopy and photoemission electron microscopy. The structure, composition, and three-dimensional morphology of these particles are revealed at near-atomic resolution. In situ heating and cooling experiments uncover unique thermodynamic behaviours, such as nanowire breakup, alloying, and structural inversion, while studies on beam-induced effects expose atomic displacements and radiolysis-driven chemistry. Our investigations include the stability of a passivation of Ni, Fe, and Co cores of 2 to 3 nm diameter by a few layers of gold and the alloy formation at high temperature.
Ag@ZnO core@shell particles exhibit enhanced electron emission upon excitation of the localized surface plasmon resonance in Ag at around 3 eV.
Vanadium oxides represent a prominent materials class for catalytic applications. When deposited after clustering in helium, we have shown that V2O5 nanoparticles keep the original stoichiometry. In combination with gold doping, Janus particles of Au and V2O5 with radii of about 20 nm are identified.

M32 - Physical Vapor Deposition of Nitride Thin Films

M32 – Session 1 (Mon 21, 10:30-12:30)			
ID	Title	Speaker	Type
608	**Wurtzite Ferroelectrics for Harsh Environment Memory Applications**	Simon Fichtner	Invited talk (10:30-11:00)

Simon Fichtner (1,2) Maike Gremmel (1) Roberto Guido (3) Redwanul Islam (1) Jun Peng (2) Niklas Wolff (1) Georg Schönweger (1,2) Niklas Kyoushi (1) Dheeraj Kumar (1) Lorenz Kienle (1) Uwe Schröder (3)

(1) Kiel University
(2) Fraunhofer ISIT
(3) Namlab

As a research direction, wurtzite structured nitride ferroelectrics have seen rapid progress since their discovery in 2019 in terms of scalability, integration and fundamental understanding [1,2]. As the material class becomes more mature, harsh environment data storage and computing emerges as a commercial application target where wurtzite ferroelectrics have substantial advantages compared to competing technologies for non-volatile memory. Among these are a high maximum use temperature of > 1000°C for AlScN, large remanent polarization > 100 µC/cm^2, inherent radiation tolerance as a wide-bandgap semiconductor and good resistance against e.g. humidity and reducing atmospheres [3].
This contribution will commence by discussing the fundamental reasons that make nitride ferroelectrics with wurtzite structure particularly insensitive to the effects of temperature increase and how this manifests in their crystal structure and e.g. pyroelectric properties. In the following, recent progress on understanding major performance metrics, especially related to imprint variation and its influence on data retention will be discussed. By analyzing opposite state retention on capacitor level, we could recently demonstrate that AlScN FeRAM concepts in their present form can already surpass industrial memory standards for harsh environment memories (10 years at 150°C) [4]. On top of this, using only partial switching to store information can further boost opposite state retention to potentially millions of years at 150°C, thereby also creating an impressive margin for data retention at hundreds of °C.

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[2] S. Fichtner, M. Uehara, I. Streicher, S. Yang, J.-P. Maria, Z. Mi, S. Leone, H. Funakubo, MRS Bulletin 50, 1079 (2025)
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[4] R. Guido, M. Gremmel, T. Mikolajick, S. Fichtner, and U. Schroeder, Adv. Funct. Mater. 35, 2421793 (2025)

102	**Al(X)N-based thin films for advanced MEMS applications**	Marco Deluca	Contributed talk (11:00-11:15)

Marco Deluca (1) Balasubramanian Sundarapandian (1) Dmytro Solonenko (1) Joaquín Miranda (1) Sanjay Nayak (1) Venkata Raveendra Nallagatla (1) Tai Nguyen (1) Nastaran Behravan (1)

(1) Silicon Austria Labs GmbH

Al(X)N substituted with Sc (Al1-xScxN, ASN) is one of the most popular thin film materials for piezoelectric micro-electromechanical system (MEMS) devices. One of the main challenges is to tailor composition and microstructure of ASN to achieve piezoelectric properties suitable for actuator applications. In this work, we will showcase some approaches to enhance the piezoelectric performance of ASN either by improving the crystal quality or by designing tailored multilayer thin film stacks. In particular, we will show that by employing carefully optimized sputtering processes and suitable buffer layers and electrode designs, Al0.64Sc0.36N multilayer thin films achieve excellent piezoelectric properties, making them a valid alternative to lead-based materials for piezoMEMS. Using a compositionally graded approach, we were also able to tailor the ferroelectric imprint of AlScN thin films, which is relevant to implementation as bimorph actuator or as ferroelectric memory. Furthermore, by employing a mixed experimental-computational approach, we are also exploring alternative AlN-based alloys (e.g. AlYN), which may lead to replacing the critical element Sc, thus enhancing the sustainability and EU strategic autonomy for this class of materials.

280	**Heterovalent Alloying of AlN-based Thin Films**	Wayne Yeo	Contributed talk (11:15-11:30)

Wayne Yeo (1) Geoff Brennecka (1) Keisuke Yazawa (2)

(1) Colorado School of Mines
(2) National Laboratory of the Rockies

Thin film aluminum nitride (AlN) and its derivative alloys are widely utilized in lead-free piezoelectric microelectromechanical systems due to its high acoustic velocity, deposition process reproducibility and chemical compatibility with semiconductor technologies. While (Al, Sc)N is by far the most used alloy, there is significant push to find a replacement for Sc due to supply concerns.
In this work, we investigate a class of heterovalently alloyed AlN-based thin films synthesized by reactive magnetron sputtering, focusing on Al–Sc–O–N, Al–Hf–N, and Al–Si–C–N. By systematically varying growth conditions and alloy composition, we explore the impact of non-isovalent substitution on phase stability, texture evolution, and functional properties such as dielectric and piezoelectric responses.
We present a framework linking defect chemistry, microstructure, and electrical properties. These insights are further extended to other heterovalent alloys of interest such as Al–Zr–N, highlighting the broader potential of heterovalent alloying as a potential route to engineer high-performance piezoelectric nitride thin films for next-generation acoustic resonators, sensors, and energy harvesting devices.

461	**AlYN thin films with high Y concentration using reactive magnetron sputtering**	Balasubramanian Sundarapandian	Contributed talk (11:30-11:45)

Balasubramanian Sundarapandian (1) Adrien Piot (1) Anton Lagosh (1) Marco Deluca (1) Dmytro Solonenko (1)

(1) Silicon Austria Labs GmbH

Next-generation telecommunication standards demand compact filters that can offer low acoustic loss, wide bandwidth, and steep filter skirts to enable efficient operation at high frequencies. To meet these requirements, bulk acoustic wave (BAW) resonators that combine a high quality factor (Q) factor with a high effective electro-mechanical coupling coefficient (keff2) are desired. Wurtzite aluminum scandium nitride (AlScN) due to its optimal piezoelectric, electrical, and thermal properties has become the industry standard for these applications. Despite these advantages, the search for alternative alloying elements has accelerated due to concerns related to the availability and cost of Sc. Yttrium (Y) has a similar valence electron configuration as Sc and hence has emerged as a promising alternative. Although mixing enthalpy calculations show that AlYN retains its wurtzite structure up to a Y concentration of 75%, experimentally this has not been achieved yet. [1,2] In this work, we tackle this limitation by engineering the seed layer to incorporate more Y into the AlYN thin film.
We deposit Al1-xYxN on Pt/SiO2/Si substrates using AlN or Al1-xYxN seed layer. Our preliminary results agree with previous reports pointing out the critical role of the seed layer [2]. The use of the graded Al1-xYxN seed layer significantly improves the crystalline quality of Al0.85Y0.15N as well as the AlN seed layer of different thicknesses. Based on these findings, we further optimize Al1-xYxN film quality by engineering the concentration and thickness of graded Al1-xYxN seed layer aimed to enhance structural and piezoelectric properties.

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[2] Solonenko, Dmytro, et al. "AlYN thin films with high Y content: Microstructure and performance." physica status solidi (RRL)–Rapid Research Letters 17.10 (2023): 2300193.

352	**Impact of AlN Buffer Layer Growth on the Quality of Mo(110) Thin Films for Acoustic Resonator Applications**	Tamara Terzic	Contributed talk (11:45-12:00)

Tamara Terzic (1) Jürgen Bläsing (2) Armin Dadgar (2) Florian Hörich (2) Dmytro Solonenko (1) André Strittmatter (2)

(1) Silicon Austria Labs GmbH
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Molybdenum (Mo) thin films find application as a bottom electrode material for acoustic resonators due to their favorable acoustic and physical properties. For subsequent overgrowth with piezoelectric materials such as AlN, which are necessary for acoustic resonators, high quality and low roughness of Mo (110) thin films are essential. Direct deposition of Mo on silicon (Si) is challenging, as interfacial reactions can lead to the formation of Mo-Si compounds, degrading the film quality and negatively impacting the growth of any subsequent functional layers. One method to suppress this compound formation is the use of a buffer layer, such as aluminum nitride (AlN), which is also known to promote (110) oriented growth of Mo. In this work, an optimized process for the deposition of highly crystalline Mo with low roughness on AlN (0002) buffer layers using pulsed DC magnetron sputtering is presented. Two differently grown types of AlN (0002) buffers were investigated. The first approach relies on an N_2 based growth process, leading to the common columnar type of AlN growth with a roughness of 2 nm RMS. The second approach uses a two-step growth process, where an initial N_2-grown AlN template is followed by NH_3-based growth, enhancing lateral growth and column coalescence, leading to a reduction of roughness to 0.35 nm RMS. Overgrowing both these templates with Mo leads to drastically different results: While the overgrowth of the N_2 grown AlN with Mo results in RC FWHM of 0.74° and a roughness close to 2 nm RMS, the overgrowth of the bilayer AlN leads to RC FWHM of 0.35° and roughness beneath 0.5 nm RMS. Using this Si-AlN-Mo template, subsequent high quality AlN growth resulted in an outstanding RC FWHM of 0.74° and an RMS roughness of 1.9 nm. These results show the importance of AlN buffer layers for achieving high-quality Mo electrodes, providing a suitable template for acoustic resonator structures.

M33 - Particle Beams for Material Modification and Analysis

M33 – Session 1 (Wed 23, 16:00-18:15, Chair: Constance Toulouse)			
ID	Title	Speaker	Type
360	**New aspects for nanoscale material evolutions under focused beams**	Stéphane Guillous	Invited talk (16:00-16:30)

Stéphane Guillous (1) Etienne Talbot (2) Adam Ockovic (1) Mathieu Lalande (3) Yann Doublet (1) Kilian Mouchel (1) Eric Giglio (1) Fabrice Gourbilleau (1) Henning Lebius (1) Pavel Loïko (1) Vincent Pacary (1) Mamour Sall (1) Clara Grygiel (1)

(1) Normandie Univ, ENSICAEN, UNICAEN, CEA, CNRS, CIMAP, UMR 6252, BP 5133, F- 14070 Caen Cedex 05, France
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This study explores the effects of localized modifications induced by micrometric ion and electron beams. Using our unique state-of-the-art PELIICAEN set-up [1,2], our work sheds light on innovative surface structuring phenomena through the control of local disorder, charge deposition and deposited power density. These transformations, resulting from complex interactions between beam and substrate, include defect accumulation, diffusion, atomic redistribution and local modification of chemical bonds.
The experimental approach relies on precise control of the flux, fluence and energy parameters of focused charged particle beams, enabling the nature and extent of the induced modifications to be finely tuned. New aspects of interpretation of the observed phenomena will be addressed to provide detailed insight into the underlying mechanisms, paving the way for a better understanding of the processes involved in the micro-nano-structuring of materials. We specifically illustrate the feasibility of generating surface protrusions on a material in a controlled manner by element implantation and defect creation. By adjusting the parameters of the focused beams, we control parameters such as local temperature elevation, charge accumulation and the coalescence of implanted elements, facilitating the formation of gas-filled hollow structures. In an ultra-high vacuum environment (10^{-9} mbar), we demonstrate the feasibility of producing quasi-spherical hollow structures measuring 1 µm in diameter in HOPG which contain implanted elements, and possess walls thicknesses of less than 10 nm, alongside structures nearly 3 µm in height obtained in silicon. Local cathodoluminescence properties induced by the creation of these structures will be discussed.
The results obtained demonstrate the potential of these techniques for nano-fabrication and surface engineering, offering tailor-made solutions for the development of high-performance devices. This study enhances comprehension of beam-matter interactions, and offers new perspectives for integrating these processes into technology applications.

714	**Functionalising 2D materials with ultra-low energy ions**	Harriet Åhlgren	Invited talk (16:30-17:00)

Harriet Åhlgren (1)

(1) Uppsala University

2D membranes are promising building blocks in various fields, but their advanced use often requires functionalisation of their surface and the modification of their physiochemical properties. Functionalisation can be achieved with defects and the incorporation of foreign atomic species. Various methods are available for this, but major challenges still lay in the control of the defect types and their concentrations. Ion irradiation at ultra-low energies (< 100 eV) offers a powerful tool to create modifications with controlled type and concentration in 2D materials by adjusting the kinetic energy of the ion and the exact number of the ions.
In this talk, I will discuss our recent efforts in applying this methodology to functionalise and manipulate 2D materials. Specifically, I will review our recent results on introducing substitutional metal atoms in graphene [1,2], and how these functional sites can be used as anchors to build single atom thick planar metal structures (metallenes) on the graphene surface [3]. Further, I will discuss our recent work with few-layer thick MoS2 membranes, focusing on ion irradiation induced defect engineering of the 2D surface and trapping atoms in-between the membranes for electronic band structure modification [4]. Our approach encompasses both experimental and computational routes, including characterisation with atomic resolution electron microscopy and Raman spectroscopy accompanied with molecular dynamics and density functional theory calculations.

[1] Trentino,.., Åhlgren et al. Micron 184, 103667, 2024.
[2] Trentino,.., Åhlgren, 2D Materials 9, 025011, 2022.
[3] Joudi, .., Åhlgren, ACS Nano 19, 22032-22043, 2025.
[4] Nawaz, James.., Åhlgren, unpublished.

592	**Development of a setup for in situ preparation, introduction, and analysis of metallenes**	Barbara Maria Mayer	Contributed talk (17:00-17:15)

Barbara Maria Mayer (1) Dmitrii Moldarev (2) Radek Holeňák (1) Kevin Vomschee (1) Daniel Primetzhofer (1,3) Harriet Åhlgren (1,2)

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(2) Department of Physics, University of Helsinki, P.O. Box 43, FI-00014, Helsinki, Finland
(3) Tandem Laboratory, Uppsala University, Uppsala, Sweden

Metal structures with an ultimate thickness of one atomic layer (metallenes) have attracted increasing research interest due to their low dimensionality and unique properties, including ultrahigh carrier mobility and enhanced catalytic activity, making them promising candidates for electrocatalysis, sensing, and next-generation electronics [1].
However, realizing metallenes is hindered by strong metallic bonding, which favors the formation of three-dimensional clusters rather than two-dimensional structures [2]. To overcome this limitation, we plan to use ultra-low-energy (tens to hundreds of eV) ion irradiation to first introduce vacancies into graphene and then place metal atoms on the graphene surface. Vacancies serve as trapping sites for metal atoms and as strain-inducing sites, enabling the formation of new, energetically favorable phases. A similar approach has been used to create 2D gold structures on [3,4].
For reliable characterization of metallenes, it is crucial to avoid surface contamination during and after implantation. One way to obtain a clean graphene surface is to anneal it under vacuum at high temperatures [5]. However, breaking the vacuum leads to contamination buildup on the surface. The University of Uppsala's time-of-flight medium-energy ion scattering (ToF-MEIS) system offers a promising approach by connecting a MEIS chamber, used for metal implantation and quantitative sputter/recoil analysis [6], to a vacuum annealing vessel, ensuring the sample is never exposed to pressures above 10 mbar

[7]. However, as the current MEIS system only allows irradiation at energies from a few to hundreds of keV, we plan to extend the MEIS setup with a deceleration unit to bring ions into the ultra-low-energy regime. This will enable in situ cleaning, metal implantation, and ion-beam analysis of the resulting structures, allowing us to experimentally study metallenes on a new scale.

[1] Fengzhu Ren et al. 2026 Adv. Mater. 38 12683
[2] Kameyab Raza Adibi et al. 2024 Nanoscale 16 19649
[3] Wael Joudi et al. 2025 ACS Nano 19 22032
[4] Alberto Trentino et al. 2022 2D Mater. 9 025011
[5] Philipp Irschik et al. 2026 2D Mater. 13 025001
[6] Radek Holeňák et al. 2025 Vacuum 204 111343
[7] Radek Holeňák et al. 2025 Vacuum 231 113824

193	**Ion Beam Implantation of Y-Zr-O Ions at 500 °C on FeCr-Based ODS Steel: Influence of Surface Preparation Methods on Precipitate Size, Distribution, Nucleation Mechanisms, and Crystallographic Evolution Revealed by Advanced TEM (TEM, HAADF STEM/EDS) for Nuclear Structural Materials**	Manoj Kumar Rajbhar	Contributed talk (17:15-17:30)

Manoj Kumar Rajbhar (1,2) Toulouse Constance (2) Aurélie Gentils (1) Stéphanie Jublot-Leclerc (1)

(1) Université Paris-Saclay, CNRS/IN2P3, IJCLab
(2) Laboratoire CRISMAT (UMR 6508), Universite de Caen Normandie, 14050 Caen, France

Ion implantation at 500°C into bcc Fe–Cr model alloys offers a controlled non-equilibrium platform to dissect the physics of Y–Zr–O nano-oxide nucleation and evolution in oxide-dispersion strengthened (ODS) steels for nuclear applications, simultaneously delivering chemical supersaturation of low-solubility Y/Zr solutes and high-damage collision cascades within a ~100 nm surface layer that store excess free energy as mobile point defects and cascade remnants driving radiation-enhanced diffusion and heterogeneous nucleation on dislocation loops and collapse sites. Advanced TEM/STEM analysis shows that Y–Zr–O nano-oxides form through fast, non-equilibrium processes, producing different crystal structures—fluorite-type (like YSZ), pyrochlore-related, and triclinic $Y_4Zr_3O_{12}$—with distinct HRTEM/FFT patterns that reveal their atomic arrangement, along with some preferred matrix/oxide orientation relationships that reduce elastic strain energy. HAADF-STEM Z-contrast imaging reveals bright Y/Zr-enriched within precipitates that show clear Fe/Cr depletion relative to the surrounding matrix, while EDS chemical mapping and quantification establish precise Y:Zr:O stoichiometries ranging from ~1:1 to 1:3—together providing definitive proof of discrete, chemically-distinct oxide phases rather than mere solute segregation or clustering. Mechanical polishing creates surface dislocations that favor shallow nucleation (skewed profiles, broad sizes), while twin-jet electropolishing yields uniform subsurface oxides. This surface scales trap solutes or block O-transport, tuning stoichiometry. At 500°C, fast oxygen diffusion stabilizes early Y/Zr–O clusters whose structure follows local cascade geometry, not equilibrium phase diagrams.

288	**Vacuum compatible printed circuit board anodes for particle detection with electron multiplier devices**	Michael Kendler	Contributed talk (17:30-17:45)

Michael Kendler (1) Sophie Wrathall (1) Lisa Gmainer (1) Alexander Redl (1) Anna Niggas (1) Philippe Roncin (2) Richard Wilhelm (1)

(1) TU Wien
(2) University of Paris-Saclay

Electron signal amplifiers such as microchannel plates (MCPs) or channeltron electron multipliers (CEMs) play an important role in particle detection and beam diagnostics across a wide range of applications in industry and R&D. To collect the amplified signals, various types of anodes are used with these electron multipliers to extract spatial and/or temporal information from the charge clouds generated by particle impacts [1].
We present a new anode design based on ultra-high-vacuum-compatible polyimide laminates used as a substrate for printed circuit board (PCB) layouts [2]. This approach enables excellent particle timing performance due to embedded polyimide-core decoupling capacitors and impedance-matched signal transmission lines [3]. While most anode designs rely on external signal decoupling circuits, we employ an in-vacuo high-pass filter to extract fast timing signals with higher bandwidth and improved signal-to- noise ratio. The method allows for a customized layout of parallel-operated segmented anode patches to differentiate impact locations, e.g., with an MCP.
The flexible nature of the laminates allows for flat waveguide strips and the ability to bend parts of the PCB in arbitrary directions without mechanical or electrical failure. These printed transmission lines are better suited for signal extraction in small vacuum installations compared to rigid coaxial cables, which are typically required for high-frequency applications. This technology platform paves the way for compact, tailor-made, or more complex vacuum circuits.

[1] T. Iijima, Nucl. Instrum. Meth. A 639, 137 (2011).
[2] M. Kendler et al., accepted in Rev. Sci. Instrum. (2026).
[3] P. Wurz and L. Gubler, Rev. Sci. Instrum. 65, 871 (1994).

456	**Investigating the Formation of Carbon Nanomembranes (CNMs) with Single and Double Electron Spectroscopy**	Felix Blödorn	Contributed talk (17:45-18:00)

Felix Blödorn (1) Anna Niggas (1) Richard Arthur Wilhelm (1)

(1) Institut für angewandte Physik, TU Wien

The electron-induced crosslinking of self-assembled monolayers (SAMs) on surfaces can lead to the formation of mechanically stable carbon nanomembranes (CNMs). These membranes have applications in waterfiltration and can be functionalised to be used in biosensing [3]. The formation mechanism from a SAM to a CNM is still elusive [1] and the atomistic structure of the final CNM is also not accessible with most common experimental methods (TEM, AFM, XRD) [2].
We use slow electrons ($\lesssim 100$ eV) to crosslink the SAM in-situ and monitor the crosslinking by Reflective Electron Energy Loss Spectroscopy (REELS) at various probing energies. Furthermore, we performed electron pair spectroscopy, where we detect the scattered primary electron in coincidence with a emitted secondary electron before and after crosslinking.

The REEL spectra show a gradual change of specific energy loss features, which can be linked to the disintegration of the molecular structure of the SAM. The pair emission spectroscopy allows us to correlate these specific loss features to energy dissipation branches with and without secondary electron emission. We put our data in context to findings of ion-beam transmission spectroscopy of CNMs and model calculations for possible atomistic CNM structures [2].

[1] C. Neumann et al, Faraday Discuss., 227:61–79, 2021.
[2] F. Vukovic et al, J. Phys. Chem. C, 130(11):4244–4255, 2026.
[3] A. Turchanin et al, Adv. Mater., 28(29):6075–6103, 2016

626	**Low-Energy Electron Emission from Layered Materials**	Anna Niggas	Contributed talk (18:00-18:15)

Anna Niggas (1) Maosheng Hao (2) Felix Blödorn (1) Florian Simperl (1) Alessandra Bellissimo (3) Joachim Burgdörfer (2) Florian Libisch (2) Wolfgang S.M. Werner (1) Richard A. Wilhelm (1)

(1) TU Wien, Institute of Applied Physics, Vienna, Austria
(2) TU Wien, Institute for Theoretical Physics, Vienna, Austria
(3) TU Wien, Institute of Photonics, Vienna, Austria

Secondary electron emission is fundamental to electron-surface interactions, underpinning technologies from microscopy to semiconductor processing. Yet the microscopic pathways driving low-energy emission (<20 eV) remain elusive. In particular, secondary electron spectra are often simply described as broad and featureless as a result of multiple scattering, concealing the underlying physics. Coincidencespectroscopy can help to overcome this challenge by detecting electron pairs from the same scattering event, e.g. a scattered primary electron after interaction with the material and a secondary electron. This approach allows us to study otherwise hidden spectral features in the secondary electron spectrum.
We have applied electron pair emission spectroscopy to tracethe evolution of secondary emission across the dimensional transition from bulk graphite through bilayer to monolayer graphene. Remarkably, we uncover layer-dependent features: the prominent 3.3 eV resonance (often termed the X peak [1]) in graphite, another peak at 7.7 eV dominating the bilayer graphene spectrum, and no distinct spectral feature in monolayer graphene. These signatures defy a simple explanation in terms of just the surface density of states alone. Instead, density functional theory calculations reveal Feshbach-type resonances of quasi-bound above-vacuum states — so-called doorway states — that couple material excitations to the continuum [2,3].
In this contribution we discuss how low-energy electron emission becomes a sensitive probe of material-specific electronic structure, with coincidence spectroscopy serving as the key that unlocks its full diagnostic potential.

[1] H. Yamane et al. Phys. Rev. B 64 113407 (2001)
[2] W.S.M. Werner et al. Phys. Rev. Lett. 125 196603 (2020)
[3] A. Niggas et al. Phys. Rev. Lett. 135 166401 (2025)

M33 – Session 2 (Thu 24, 16:00-18:00, Chair: Anna Niggas)

ID	Title	Speaker	Type
500	**Atom and ion irradiation of graphene: disentangling elastic from inelastic scattering and the role of phonons**	Toma Susi	Invited talk (16:00-16:30)

Toma Susi (1) Christian Brand (2) Maxime Debiossac (2) Carina Kanitz (2) Filip Vuković (3) Richard Wilhelm (3) Vladimír Zobač (1)

(1) University of Vienna
(2) German Aerospace Center (DLR)
(3) TU Wien

Graphene provides the thinnest possible diffraction grating for atom and ion transmission, providing an ideal robust model system for studying the fundamental physics of energy and momentum transfer, and the loss of coherence. Understanding atomic-scale details is only possible with the help of first-principles simulations capable of describing energy loss, which is feasible with the help of time-dependent density functional theory. Our implementation of LCAO Ehrenfest molecular dynamics (ED) method within the projector augmented-wave code GPAW yields satisfactory accuracy at a much-reduced computational cost, which is particularly useful for modeling irradiation processes that require large amounts of vacuum in the simulation cell [1].
After the first demonstration of atom diffraction in transmission through a crystal [2], new measurements have now been performed with an improved graphene sample featuring large monocrystalline domains comparable in size to the beam diameter. In these experiments, the shape of the diffraction pattern is largely determined by the lattice at equilibrium whereas vibrationally-induced distortions are treated perturbatively. By including a model of the target lattice incorporating thermally diffuse scattering via phonon normal modes, we show that the perturbative approach does not hold for helium diffracted at kiloelectronvolt energy through freestanding single-layer graphene. In this case, we enter a new regime of strong coupling, where the projectile strongly interacts with the electron density of several lattice atoms simultaneously, with the weak-coupling regime is retained for atomic hydrogen diffraction [3].
Turning then to ion transmission, the charge of an ion becomes a dynamic quantity when it is in contact with other atoms, molecules, or solids, leading to a complex coupling between stopping processes in matter. We perform experimentally-benchmarked Ehrenfest dynamics simulations of neutral Xe and Xe^{12+} ions transmitted through freestanding single-layer of graphene to reveal the synergy between nuclear and electronic stopping. Importantly, momentum transfer from phonons excludes the high-symmetry bond-center impact parameter from the small acceptance angle of the ion analyzer. Relative to neutral projectiles, ions exert an enhanced nuclear energy transfer, and exhibit non-trivial electronic energy losses. This can result in greater electronic stopping for neutral projectiles compared to ions under certain conditions. Our findings challenge the typical notion that ion stopping force is merely the sum of independent nuclear and electronic stopping components [4].

Funding by the Austrian Science Fund (FWF) via grant P 36264-N is gratefully acknowledged.

218	**Slow highly charged ions as a tool for tailoring strongly correlated quantum materials**	Richard Wilhelm	Invited talk (16:30-17:00)

Anna Niggas (1) Richard Wilhelm (1) Jens Buck (2) Kai Rossnagel (2) Victoria Vojtech (1) Filip Vuković (1)

(1) TU Wien
(2) DESY

Strong correlations in materials are facilitated through electron-electron or electron-phonon interactions and lead to phenomena beyond the single-active-electron picture of traditional solid-state physics. In the prototypical material 1T-TaS2, these interactions lead to a specific surface reconstruction at low temperatures closely linked to a charge density wave. At low temperatures, the surface of 1T-TaS2 shows a correlation band gap, while at higher temperatures the surface is metallic [1].
As the specific electronic and structural properties of this class of Peierls-Mott transition materials are defined by electron-electron and -phonon interactions, electronic excitations may weaken the surface stability and allow for transitions into different phases. Such phases, which cannot be reached in thermodynamic equilibrium, are particularly interesting for novel application for electronic devices [2].
We utilize the strong electronic interaction of highly charged ions with a surface to induce a chiral switch in the commensurate charge density wave phase at 50K of 1T-TaS2. By monitoring the evolution of the surface band structure under ion bombardment in operando with angle-resolved photoelectron spectroscopy, we observe a gradual change of the surface (2D) chirality. We explain our findings by the ion destabilizing the electronic structure of the surface upon neutralization. At the same time, introducing single atomic displacements breaks the surface symmetry, and surface atoms are rearranged in the opposite chirality upon energy dissipation [3].
Our results show that the electronic interaction of ions can be used to tailor surfaces which are governed by strong correlations. This opens the door towards the rich toolbox of ion beam physics for quantum materials.

[1] K. Rossnagel, J. Phys. Cond. Matter 26 (2011) 213001.
[2] L. Stojchevska, Science 344 (2014) 6180.
[3] A. Niggas et al., Nano Lett. 26 (2026) 2002.

368	**Revealing charge fractions in LEIS from comparison to scattering-event-resolved simulations**	Johannes Brötzner	Contributed talk (17:00-17:15)

Johannes Brötzner (1) Matthias Kogler (1) Lukas Kalchgruber (1) Paul S. Szabo (2) Andreas Nenning (3) Andreas Mutzke (4) Hans Hofsäss (5) Markus Valtiner (1) Richard Wilhelm (1)

(1) TU Wien, Institute of Applied Physics
(2) University of California Berkeley, Space Sciences Laboratory
(3) TU Wien, Institute of Chemical Technologies and Analytics
(4) Max Planck Institute for Plasma Physics
(5) Universität Göttingen, II. Physikalisches Institut

Low-energy ion scattering (LEIS) is an ion beam analysis technique with utmost surface sensitivity [1]. When used with electrostatic analysers for ion detection (esaLEIS), the resulting high solid-angle coverage allows for spectra acquisition in short time scales and at low sample exposure to the incoming ion flux. However, in esaLEIS, only charged particles are detected, limiting quantitative analyses unless the charge fractions of probing ions are known.
Here, we present a combined experimental and numerical approach to analyse LEIS spectra obtained from He^+ scattering off a $CaSiO_3$ sample with energies from 1–3 keV. Experiments were carried out using a commercially available setup (ionTOF Qtac). Simulations were performed with the binary collision approximation codes SDTrimSP [2] and IMINTDYN [3]. The former enables the calculation of the equilibrium surface composition after sputter cleaning, while the latter is capable of directly calculating LEIS spectra under consideration of the experiment geometry. Furthermore, it can separate the simulated spectra by scattering partner (sample species) and scattering type (whether the ion scattered once, twice, or multiple times).
While the experimental spectra contain only charged ions, the simulations do not account for neutralisation and/or re-ionisation processes. A comparison therefore enables to extract the charge fraction of the probing He after scattering. The singly scattered particles make up most of the characteristic peaks in the LEIS spectra used for elemental identification. The double and multiple scattering events, while suppressed by roughly an order of magnitude, determine the shape of the spectral background. Beyond this deeper understanding of the spectral shapes, our results on the charge fra-ctions potentially aid future quantification of samples with similar chemical environments in LEIS.

[1] H.H. Brongersma et al., Surf. Sci. Rep. 62 (2007) 63–109.
[2] A. Mutzke et al., (2019).
[3] H. Hofsäss, A. Stegmaier, Nucl. Instrum. Methods Phys. Res. B 517 (2022) 49–62.

349	**Picosecond Laser-Stimulated Ion Pulses from Tungsten Nanotips for Time-Resolved Low-Energy Ion-Scattering**	Alexander Redl	Contributed talk (17:15-17:30)

Alexander Redl (1) Lisa Gmainer (1) Markus Goldberger (1) Michael Kendler (1) Richard Wilhelm (1)

(1) TU Wien

Ultrashort ion pulses enable time-resolved investigations of ion-surface interactions on picosecond timescales. Laser-stimulated desorption (LSD) from metallic nanotips has emerged as a promising approach for generating such pulses, combining nanometric spatial confinement with strong electrostatic field enhancement. We present recent progress in the characterization and optimization of a sub-100 picosecond ion source and outline its application in a novel time-of-flight-resolved low-energy ion scattering (TOF-LEIS) experiment.
The source consists of an electrochemically etched tungsten nanotip with a tip radius between 15-100 nm, biased to +6.5 kV. Femtosecond ultraviolet laser pulses induce the desorption and ionization of arbitrarily selectable adsorbed species, producing ions with sub-10 keV kinetic energies. TOF measurements reveal pulse durations of 84 ps for hydrogen ions with intrinsic synchronization to the driving laser [1].
Utilizing charged-particle trajectory simulations with the SIMION software package [2], the experimentally observed TOF spectra were quantitatively reproduced. The simulations demonstrate that the ion pulse widths are dominated by transport-induced temporal dispersion rather than intrinsic desorption dynamics. Geometric acceptance and trajectory filtering are identified as the primary factors for determining the temporal resolution, providing clear guidelines for source optimization towards the single digit picosecond regime.

Building on these insights, we are developing a TOF-resolved LEIS pump–probe experiment that exploits the inherent synchronization between the ultrashort ion pulses and the femtosecond laser. In this scheme, laser-induced and reversible surface modifications are probed by delayed ion pulses, extracting information on transient changes in surface stoichiometry and atomistic structure.

[1] A. Redl, et al., Physical Review Research 7, 043317 (2025)
[2] D. J. Manura and D. A. Dahl, Simion software package v8.1.2 (2014)

147	**Atomic-Scale Characterization of Point Defects in Complex Oxides**	Elena Martina Unterleutner	Contributed talk (17:30-17:45)

Elena Martina Unterleutner (1) Benedikt Haas (2) Anton Gladyshev (2) Mairi McCauley (2) Luka Wibmer (3) Markus Aichhorn (3) Ferdinand Hofer (1) Christoph T. Koch (2) Gerald Kothleitner (1) Daniel Knez (1)

(1) Institute of Electron Microscopy and Nanoanalysis, Graz University of Technology, Graz, Austria
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(3) Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria

Defect engineering is an important strategy for tuning the electronic and magnetic properties of complex oxides. Therefore, it is essential to understand atomic-scale defects, such as dopants and vacancies, in complex oxides like SrTiO (STO). However, linking the microscopic properties of individual point defects to macroscopic material behavior remains challenging. Although first-principles density functional theory (DFT) provides the structural and electronic basis needed to interpret advanced electron microscopy data and predict bulk functionality, reliable defect characterization and single-atom sensitivity in the bulk are often limited by spatial resolution, signal sensitivity, and experimental stability.
To address this, we conducted atomic-resolution momentum-resolved scanning transmission electron microscopy, mostly called 4D-STEM [1], experiments on STO doped with 0.5 wt% Ta using a Nion HERMES microscope operated at 60 kV with a semi-convergence angle of 36 mrad. Ultrathin samples (less than 6 nm), prepared by wedge polishing and characterized by neural network-assisted PACBED analysis [2], were crucial for reliable defect detection. [3] DFT calculations [4] were used to determine relaxed structures of Ta dopants and associated Sr vacancies. These structures were then used in multislice simulations [5] to optimize the experimental conditions and predict defect-induced changes in the angular scattering distribution. [6]
We demonstrate that sub-ångström atomic displacements generate distinctive diffuse Huang scattering [7] that significantly impacts the momentum-resolved 4D-STEM signal. By incorporating these distortions into the simulations, we identify defect-specific scattering signatures and design virtual detectors that enhance sensitivity to individual point defects.
By combining DFT-derived defect structures, multislice simulations, and 4D-STEM, we establish a robust framework for detecting and characterizing individual point defects in complex oxides and other functional materials.

[1] Colin Ophus. “Four-Dimensional Scanning Transmission Electron Microscopy (4D-STEM): From Scanning Nanodiffraction to Ptychography and Beyond”, Microscopy and Microanalysis 25.3 (2019): 563–582.
[2] Oberaigner, Michael, et al. "Online thickness determination with position averaged convergent beam electron diffraction using convolutional neural networks." Microscopy and Microanalysis 29.1 (2023): 427-436.
[3] Mittal, Anudha, and K. Andre Mkhoyan. "Limits in detecting an individual dopant atom embedded in a crystal." Ultramicroscopy 111.8 (2011): 1101-1110.
[4] Volker Blum, Ralf Gehrke, Felix Hanke, Paula Havu, Ville Havu, Xinguo Ren, Karsten Reuter, and Matthias Scheffler, “Ab Initio Molecular Simulations with Numeric Atom-Centered Orbitals”, Computer Physics Communications 180 (2009): 2175-2196.
[5] Madsen, Jacob, and Toma Susi. "The abTEM code: transmission electron microscopy from first principles." Open Research Europe 1 (2021): 24.
[6] Rafael Fritz. „Quantitative Untersuchungen der Zusammensetzung von kubischen III/V-Verbindungshalbleitern mittels HAADF-STEM“, PhD Thesis, Philipps-Universität Marburg (2013)
[7] Huang, Kun. "X-ray reflexions from dilute solid solutions." Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences 190.1020 (1947): 102-117.

257	**Temperature distribution profile in metal surfaces irradiated by slow highly charged ions**	Milena Majkić	Contributed talk (17:45-18:00)

Milena Majkić (1)

(1) Faculty of Technical Sciences, University of Priština-Kosovska Mitrovica, Serbia

The surface modifications induced by the impact of slow highly charged ions (HCI), in the form of nano-sized features such as hillocks, holes or craters, are influenced by various parameters, most notably the ion kinetic energy (velocity) and potential energy (charge state) [1]. Understanding the mechanisms underlying these surface modifications is crucial for applications in defect engineering, ion-beam processing, ion-beam analysis, and requires essential theoretical insights into the nanostructure formation process.
When slow highly charged ions impinge on a solid surface, they deposit their energy primarily into the electronic subsystem, leading to intense electronic excitation. This energy is subsequently transferred to the atomic subsystem via electron- phonon coupling, resulting in a transient increase in local energy density and a corresponding rise in lattice temperature within the impact region, which ultimately leads to surface modification.
The temperature evolution in metal surfaces irradiated with HCI has been investigated through the interplay between the two-step cohesive energy model [2] and an analytical thermal spike model [3]. The combined model indicates that the energy density associated with the velocity effect determines the type of nanostructure formed [4]. Hillocks are formed at lower ion velocities, where the energy density is lower, and craters emerge at higher velocities, where the energy density becomes significantly larger. The dependence of the temperature distribution profile on ion velocity and charge state has also been analyzed. These results demonstrate that the coupled cohesive energy and analytical thermal spike framework provides valuable insight into the mechanisms governing velocity-dependent surface modification induced by slow highly charged ions.

[1] F. Aumayr et al., J. Phys.: Condens. Matter 23, 39 (2011)
[2] N. N. Nedeljković, M. D. Majkić, D. Banas, I. Stabrawa, Vacuum 224 113136 (2024)
[3] G. Szenes, Radiation Effects and Defects in Solids 175 (3-4) (2020) 241–256.
[4] M. D. Majkić, Material Science and Engineering: B, to be published

M33 – Session 3 (Fri 25, 10:30-12:30, Chair: Denise Erb)			
ID	Title	Speaker	Type
417	**Non-Equilibrium Pattern Formation on Surfaces under Ion Beam Irradiation**	Stefan Facsko	Invited talk (10:30-11:00)

Stefan Facsko (1)

(1) Ion Beam Center, Helmholtz-Zentrum Dresden-Rossendorf

Low- and medium-energy ion beam irradiation of surfaces induces a variety of nanoscale morphologies, depending on the irradiation conditions [1]. Under specific conditions, hexagonally ordered dot or pit arrays, checkerboard patterns, and periodic ripple structures oriented either perpendicular or parallel to the ion beam direction can form spontaneously during continuous surface erosion by ion sputtering.
On amorphous surfaces, pattern formation is primarily governed by the interplay between roughening mechanisms, e.g., curvature-dependent sputtering, ballistic mass redistribution, and composition changes in multicomponent materials—and smoothing mechanisms, including surface diffusion and viscous flow.
An additional surface instability emerges above the recrystallization temperature, where ion-induced bulk defects are dynamically annealed and amorphization is suppressed. In this regime, the diffusion of ion-induced vacancies and adatoms on crystalline surfaces is influenced by the Ehrlich–Schwoebel (ES) barrier, i.e., an additional energy barrier for interlayer mass transport across terrace steps. As a result, vacancies and adatoms become trapped on terraces and can nucleate into extended pits or islands, respectively [2].
Patterns formed in this so-called “reverse epitaxy” regime exhibit well-defined crystalline facets, and their symmetry reflects the underlying crystal structure. Nevertheless, ballistic effects can still contribute significantly to morphology evolution on crystalline surfaces. This has been demonstrated for high-temperature irradiation at oblique incidence angles [3], as well as for normal incidence in the intermediate regime between checkerboard and isotropic patterns [4].
The fundamental understanding of surface pattern formation under these non-equilibrium conditions is already well advanced. Atomistic simulations, such as molecular dynamics (MD) and kinetic Monte Carlo (kMC), as well as continuum modeling approaches, successfully reproduce most experimental observations. In recent years, continuum models have been further refined, achieving increasing predictive capability for both amorphous and crystalline surfaces.

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[2] X. Ou, K.-H. Heinig, R. Hübner, J. Grenzer, X. Wang, M. Helm, J. Fassbender, and S. Facsko, Nanoscale 7, 18928 (2015).
[3] D. Erb, R. de Schultz, A. Ilinov, K. Nordlund, R. M. Bradley, and S. Facsko, Phys Rev B 102, 165422 (2020).
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634	**Learning Predictive Dynamics of Ion-Irradiated Surfaces from Sparse Data**	Miguel Sequeira	Invited talk (11:00-11:30)

Miguel Sequeira (1) Denise Erb (1) Stefan Facsko (1)

(1) Helmholtz-Zentrum Dresden-Rossendorf (HZDR)

Instability-driven pattern formation appears across many nonequilibrium systems, from nanoscale surfaces to larger-scale natural patterns. In the ion-beam community, decades of experiments have revealed a rich variety of surface morphologies, from ripples and dots to faceted structures, and continuum theories can reproduce many of these patterns qualitatively. Yet turning a continuum equation into a quantitatively predictive tool for a specific experiment remains difficult. The evolution laws assume competing mechanisms, such as curvature-dependent erosion, mass redistribution, diffusion, and step-edge barriers, whose strengths are hard to disentangle from sparse, noisy, and misregistered ex situ measurements. Physics-informed neural networks (PINNs) offer a route to closing this theory-experiment gap.
Here, we present an inverse solver that couples a PINN, that recovers the surface dynamics, with a tandem network that accounts for the measurement model. Specifically, we demonstrate the method using just six ex situ atomic force microscopy snapshots of an unstable Ge surface under ion irradiation. The method recovers the full nonlinear evolution equation and turns it into a quantitatively predictive tool. The response of unseen surfaces to ion irradiation can now be predicted with nanometre accuracy. The inferred model can be interpolated beyond the measured spatiotemporal resolution, revealing the continuous transition between experimental snapshots and approaching atomic-scale detail consistent with electron microscopy. Finally, we discuss what these results imply for predictive modelling of instabilities and for bridging experiments with predictive continuum models.

551	**The role of defects in ion induced β-Ga_2O_3 to γ-Ga_2O_3 conversion**	Gregor Hlawacek	Contributed talk (11:30-11:45)

Umutcan Bektas (1) Réne Hübner (1) Maciej Oskar Liedke (1) Nico Klingner (1) Gregor Hlawacek (1)

(1) Helmholtz-Zentrum Dresden-Rossendorf

Gallium oxide (Ga_2O_3) is a highly versatile material with applications in power electronics, optoelectronics, and battery technologies. Among its polymorphs, monoclinic β - Ga_2O_3 is the most chemically and thermally stable phase. However, controlling the metastable polymorph phases remains challenging, and fabrication technologies for nanoscale structures are still under development. This study aims to enhance the understanding of polymorph conversion mechanisms and to establish novel fabrication techniques for single-phase polymorph films, buried layers, multilayers, and various nanostructures of Ga_2O_3.
We investigate β - Ga_2O_3 samples irradiated with different ions and fluences, as well as α - and κ - Ga_2O_3 thin films. Broad beam (BB) ion irradiation was employed to induce phase transformations in the near-surface region. The irradiated samples were characterized using transmission electron microscopy (TEM) and X-ray diffraction (XRD) to analyze structural changes. Complementary experiments using Positron Annihilation Lifetime Spectroscopy (PALS) and Doppler Broadening Variable Energy Positron Annihilation Spectroscopy (DB-VEPAS) provided insights into defect types and concentrations.
Our results reveal the evolution of defect types and densities based on DB-VEPAS and positron lifetime measurements. During the phase transition from β - to γ - Ga_2O_3, a significant reduction in positron trapping sites is observed, indicating a decrease in defect density in the newly formed γ - Ga_2O_3 layer, consistent with the high radiation hardness of Ga_2O_3. Additionally, we employed Neon-based helium ion microscopy to investigate the minimal achievable polymorph feature size, producing γ - Ga_2O_3 lines as narrow as 20 nm. The lateral dimensions and shape of the observed γ regions are in excellent agreement with SRIM and TRIDYN collision cascade simulations, directly confirming the defect densities and ion fluences employed in both the FIB patterning and the PAS characterisation.

This work is supported by the m-era.net project GoFIB and funded by the Saxonian government. Additional support from the COST Action CA19140 FIT4NANO is gratefully acknowledged.

524	**Ion Beam Shaping of Catalytic Nanoparticles**	Sophie Wrathall	Contributed talk (11:45-12:00)

Sophie Wrathall (1) Noelia Barrabés Rabanal (1) Aleix Comas Vives (1) Daniela Klampfl (1) Hector Prats (1) Itzi Giselle (1) Soto Rodriguez (1) Richard Wilhelm (1)

(1) TU Wien

Metallic nanoparticles can be powerful catalysts for reactions such as the water gas shift reaction, which converts steam and CO to H_2 and CO_2 [1]. Depending on their composition, size, shape, and surface area, different nanoparticles exhibit different catalytic properties [2].
We investigated the shaping of spherical AuCu particles with 10 nm diameter using 2 keV Ar+ beams. This was done both through simulations using the binary collision approximation code SDTrimSP-3D, and experimentally, by comparing atomic force microscopy (AFM) images before and after irradiation with fluences of 0.5 ions/Å^2 and 1.0 ions/Å^2.
Simulation results show the top half of the particles eroded into a conical shape at fluences between 0.5 ions/Å^2 and 1.0 ions/Å^2. Beyond 2.0 ions/Å^2, the nanoparticles are eroded almost completely. Additionally, SDTrimSP-3D simulates changes in composition created by irradiation, predicting an enrichment of Au at the surface of the particles. AFM images are used to track the heights of the irradiated particles and those coincided well with the SDTrimSP-3D results.

[1] C. Ratnasamy and J. P. Wagner, „Water gas shift catalysis," Catalysis Reviews, vol. 51, p. 325–440, 2009.
[2] T. Ishida, T. Murayama, A. Taketoshi and M. Haruta, „Importance of Size and Contact Structure of Gold Nanoparticles for the Genesis of Unique Catalytic Processes," Chemical Reviews, vol. 120, pp. 405-408, 2020.

129	**Defect engineering for oxide thin films by ion irradiation**	Shengqiang Zhou	Contributed talk (12:00-12:15)

Shengqiang Zhou (1)

(1) Helmholtz-Zentrum Dresden-Rossendorf

Complex oxides host a multitude of novel phenomena in condensed matter physics, such as various forms of multiferroicity, colossal magnetoresistance, quantum magnetism, and superconductivity. This is largely due to the strong correlation between charge, spin, orbital, and lattice parameters. Specifically, tilting the delicate energy balance in lattice interactions and kinetics, achieved by temperature, strain, or chemical doping, can result in significant modifications in these materials [1]. In this context, defect engineering by ion irradiation, which can introduce strain and electronic disorder, has emerged as a powerful technique to fine-tune complex phases of oxide thin films. The induced uniaxial strain, manifested as the elongation of the out-of-plane lattice spacing, is not limited to available substrates, the conventional and well-known strain engineering approach. In this contribution, we will introduce the tailoring of oxide thin films by ion irradiation, with examples including the modification of magnetic and magneto-transport properties of SrRuO3 [2, 3], and ferroelectric properties of BiFeO3 [4, 5]. The irradiated SrRuO3 films exhibit a pronounced topological Hall effect in a wide temperature range from 5 to 80 K, which can be attributed to the emergence of Dzyaloshinskii–Moriya interaction resulting from artificial inversion symmetry breaking associated with lattice defect engineering. In BiFeO3, we have obtained a super-tetragonal phase with the largest c/a ratio (~1.3) ever experimentally achieved. By controlling the ion energy, we can create a continuous in-plane charged antiphase boundaries around the implanted depth. The antiphase interface reveals a variety of atomic bonding configurations, showing the atomically sharp 180° polarization reversal across the boundary. We show that ion irradiation is a very versatile pathway for tailoring oxide functionalities, analogous to ion-implantation doping for conventional semiconductors. It is worth noting that ion beam technology has been well-developed for microelectronics. Once the principle of concept is approved, the approach can be easily scaled up and integrated into the industry production line.

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[2] C. Wang, et al., Defect-Induced Exchange Bias in a Single SrRuO3 Layer, ACS Appl. Mater. Interfaces 10, 27472 (2018).
[3] C. Wang, et al., Topological Hall Effect in Single Thick SrRuO3 Layers Induced by Defect Engineering, Adv. Electron. Mater. 6, 2000184 (2020).
[4] C. Chen, et al., Controllable defect driven symmetry change and domain structure evolution in BiFeO 3 with enhanced tetragonality, Nanoscale 11, 8110 (2019).
[5] X. Cai, et al., In-plane charged antiphase boundary and 180° domain wall in a ferroelectric film, Nature Communications 14, 8174 (2023).

132	**Accessing negative pressure states for functional property tuning through strain engineering by helium implantation**	Constance Toulouse	Contributed talk (12:15-12:30)

Constance Toulouse (1) Alfredo Blázquez Martínez (2,3) Mael Guennou (4) Peter Wei-Fan Hsu (5) Jens Kreisel (4) Jean-Pierre Locquet (5) Simon Mellaerts (5,6) Julien Varignon (1)

(1) CRISMAT, University of Caen, CNRS, ENSICAEN, France
(2) Luxembourg Institute of Science and Technology
(3) Helmholtz-Zentrum Berlin
(4) University of Luxembourg
(5) KU Leuven
(6) ETH Zürich

Strain-engineering as a means to tune and control functional properties is extensively pursued in materials science today. In particular, epitaxial strain has been shown to allow the control of multiferroic properties (magnetic and ferroeletric transitions) as well as conduction states (metal-insulator or superconducting transitions) in thin films of various materials. We propose here a new way to engineer negative strain states using helium ion implantation. Helium is a noble gas, it does not form bonds, and it implants interstitially without modifying the chemistry of the host material, inducing a volume increase that can be understood as an experimental negative pressure. In thin films, due to the in-plane clamping of the film to its subtrate, helium implantation induces an out-of-plane lattice parameter expansion continuously tunable with dose [1].
In this communication, we will show that helium implantation at low doses is able to induce important structural changes and functional properties modifications while still preserving the crystallinity of the material. We could show that in epitaxial BiFeO thin films (grown by PLD) helium implantation can trigger a transition towards the super-tetragonal polymorph, allowing for an increase in tetragonality with lattice parameterexpansion up to 8.9% on SrTiO

substrate [2]. Another study in sol-gel ceramic thin films showed that we could induce out-of-place lattice expansion of up to 3.2% without inducing structural cracking, which is unprecedented in polycrystalline films, whilealso preserving the ferroelectric properties [3]. Other materials will also be discussed, such as VO, in which we are able to tune the two metal-insulator transitions under helium implantation: the first one at low-temperature (LT MIT) from the low-temperature monoclinic insulating phase to the hexagonal metallic phase of room temperature, and the second isostructural one at room temperature (RT MIT).

[1]Guo et al., Phys. Rev. Lett., 114, 256801 (2015)
[2]Toulouse et al., Phys. Rev. Mat, 5 (2), 024404 (2021)
[3]Blázquez Martínez et al., APL Mat. 13 (2), 021111 (2025)

M33 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
194 **P074**	**Ag-Ion Irradiation Induced Micro rod formation in MoO_3 for Advanced Field Emission Application**	Manoj Kumar Rajbhar	Poster

Manoj Kumar Rajbhar (1,2) Toulouse Constance (2) Paramita Maiti (3)

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(2) Laboratoire CRISMAT (UMR 6508), Universite de Caen Normandie, 14050 Caen, France
(3) Institute of Physics, Sachivalaya Marg, Bhubaneswar 751005, Odisha, India

We report the growth of molybdenum oxide nanostructures (NSs) by low-energy silver (Ag) ion irradiation. A ≈200 nm MoO3 film was deposited on Si substrates with native oxide layer by physical vapor deposition (PVD) technique. Then, 30 KeV Ag at the fluence of 5 × 10^14 , 5 × 10^15 and 2 × 10^16 ions/cm 2 was implanted on MoO3 film. From the FESEM images, it has been observed that, films transformed to rod like structures with increasing fluence from 5 × 10^14 to 2× 10^16 ions/cm^2. X-ray photoelectron spectroscopy (XPS) measurements reveal that with increasing Ag fluence, oxygen vacancy increases, MoO 3 concentration decreases, and more and more Si substrate is getting exposed. With increasing Ag fluence, RMS roughness increases from 53 nm to 261 nm, whereas band gap decreases from 3.5 eV to 2.6 eV and local work function decreases from 5.64±0.05 eV to 4.81±0.04 eV. Field emission turn-on field decreased from 5.77 V/μm for 10 μA/cm 2 to 4.83 V/μm for as deposited film to 2 × 10^16 ions/cm^2 Ag implanted sample.Highest fluence of Ag implanted sample shows better field emitter due to rod like structures, low work function, low band gap, low turn-on field and highest filed enhancement factor (FEF). In order to validate the experimental results, extensive TRI3DYN simulation was performed to show Ag enriched rod formation, atomic densities, defect densities and roughness after Ag ion irradiation.

M34 - Soft Meets Hard – Interfaces and Interactions

M34 – Session 1 (Wed 23, 16:00-18:00, Chair: Helga Lichtenegger)			
ID	Title	Speaker	Type
76	**Multifunctional 2D Hybrid Nanomaterials for Bio- and Theranostic Applications**	Cristina Satriano	Invited talk (16:00-16:30)

Cristina Satriano (1)

(1) University of Catania

Hybrid materials composed of soft organic components and hard inorganic nanostructures exhibit emergent properties governed by their interfaces and by confinement effects at the nanoscale. Understanding and controlling these soft–hard interfaces is therefore central to designing functional materials for biomedical and bioinspired applications.
Here, we report a modular one-pot approach for the synthesis of graphene-based two-dimensional hybrid nanomaterials integrating plasmonic gold and/or palladium nanoparticles together with magnetite nanodomains. The graphene oxide scaffold acts as a flexible, chemically tunable soft interface that mediates nanoparticle organization and interactions with biomolecular environments, while the embedded inorganic domains provide optical, magnetic, catalytic, and photothermal functionalities. Comprehensive physicochemical characterization reveals how nanoparticle distribution, surface chemistry, and colloidal stability arise from the interplay between soft carbonaceous sheets and rigid inorganic nanostructures. To probe molecular processes at the bio–nano interface, multiscale simulations combining density functional theory, atomistic molecular dynamics, and coarse-grained modelling were used to investigate adsorption, orientation, and dynamic restructuring of proteins and peptides on the hybrid surfaces under confinement. Biological experiments in cancer cell models demonstrate that interfacial design directly controls cellular uptake, optical traceability, and photothermal and nanozyme-mediated activity. These results highlight how soft-matter concepts—interfacial energetics, nanoscale confinement, and hierarchical organization—can guide the rational design of multifunctional hybrid nanomaterials with tunable biological responses.

259	**Abstraction and technical principle transfer of plant tendrils to robotic grippers**	Gabriel B. Fuchs	Contributed talk (16:30-16:45)

Gabriel B. Fuchs (1) Richard W. van Nieuwenhoven (1) Ille C. Gebeshuber (1)

(1) TU Wien

Biological systems provide a rich source of functional principles that can be translated into technical designs. In this work, a plant tendril is taken as an example to demonstrate how observation, interpretation, and abstraction can lead to a realizable mechanical concept.
Starting from the geometric and functional characteristics of tendrils, a segmented compliant structure was developed that captures the essential mechanism of coiling. The system consists of a flexible backbone with fixed overall length, actuated by a tendon running along the structure. Contraction of the tendon introduces a length mismatch between tendon and backbone, leading to controlled bending. The backbone is composed of rigid segments connected by compliant joints. An angular offset between these joints, in combination with tendon actuation, results in a three-dimensional spiral that reproduces the characteristic coiling behaviour observed in plant tendrils.
In this sense, the structure represents a simple example of a soft–hard interaction: deformation arises from the interplay between compliant materials and geometrically constrained elements. A qualitative mechanical description based on bending and tendon actuation is used to interpret the resulting deformation behaviour.
The concept was realized as a 3D-printed demonstrator using polymer-based materials, combining rigid segments with flexible joint elements. Actuation is controlled by a custom-built electronic system, enabling programmable tendon contraction. The resulting device is compact and suitable for demonstration, allowing direct visualization of the coiling mechanism.

346	**Modeling the interface of graphene-based nanopores, biomolecules, and solvent**	Maria Fyta	Contributed talk (16:45-17:00)

Peijia Wei (1) Chandan Das (1) Longlong li (1) Maria Fyta (1)

(1) RWTH Aachen University

Nanopores are nanometer-sized openings in materials, which can electrophoretically drive biomolecules, such as DNA and proteins, through. This transport can be monitored in real time and detect the biomolecules by analysing the ionic current flowing through the pore in the material. The efficiency of this analysis, thus the accuracy in the biomolecule detection strongly relies on the detailed interatomic interactions within the nanopore region. This involves the interactions of the biomolecule with the material and the solvent molecules. Using computer simulations at the classical and quantum mechanical level, we model these interactions in detail in the case of ultra-thin 2D materials, as well as bulky pores threading short proteins, train a Machine learning model based on the simulation insights, and discuss the relevance to biomolecule sensing and sequencing.

353	**Characterization of the osteocyte lacuno-canalicular network in human bone**	Markus Hartmann	Contributed talk (17:00-17:15)

Markus Hartmann (1) Chloe E. Jones (1) Stéphane Blouin (1) Elisa Zamengo (1) Andrea Berzlanovich (2) Emeline Raguin (3) Peter Fratzl (3) Richard Weinkamer (3) Matthias Weinberger (4) Helga Lichtenegger (4)

(1) Ludwig Boltzmann Institute of Osteology
(2) Medizinische Universität Wien
(3) Max Planck Institute for Colloids and Interfaces
(4) Universität für Bodenkultur Wien (BOKU)

Bone is a fascinating material fulfilling mechanical, hematopoiesis, mineral storage and hormonal functions. A constant supply of nutrients and mineralization precursors is fundamental to its physiological function with the osteocyte lacuno-canalicular network (LCN) as one of the key players [1]. The osteocytes are embedded in the bone matrix with the cell body housed in lacunae and their dendritic cell processes extending in canaliculi and connecting

to other osteocytes via gap junctions. The canaliculi are long canals over several µm with diameters around 300 nm. In humans the total canalicular length adds up to $2x10^5$ km (corresponding to a density of 74 km/cm^3) leading to an enormous inner surface estimated at 215 m^2 [2,3]. In this presentation, I will show how the LCN can be measured and reconstructed in 3D using fluorescent rhodamine staining and confocal laser scanning microscopy. Measurement of human iliac crest autopsy samples from donors aged between 50 and 95 years showed that the local network density depends on tissue age, rather than on donor age [4]. Interestingly, all donors of our cohort showed local network defects, like engorged and distorted canaliculi or large overstained regions. These defects can be further characterized using high-resolution techniques. Focused ion beam-SEM investigations showed a 4-fold increase in the amount of non-mineralized tissue in defective compared to typical regions [4]. X-ray nano-holotomography measurements at the ESRF, Grenoble, confirmed these results showing that non-mineralized regions can be frequently found close to normally mineralized ones. While in the investigated cohort such mineralization defects could be found in donors of all ages, their size increased with age. This might be a contributor to the loss of bone material quality in the elderly.

[1] Raguin et al., Adv. Sci. 10, 2301231 (2023)
[2] Buenzli & Sims, Bone 75, 144 (2015)
[3] Repp et al., Bone Rep. 6, 101 (2017)
[4] Jones et al., Acta Biomater. 209, 493 (2026)

696	**Structural analysis of biological materials using Energy Dispersive Laue Diffraction**	Arno Frank	Contributed talk (17:15-17:30)

Phil Cook (1) Arno Frank (1) Klaudia Hradil (2) Dieter Ingerle (2) Helga Lichtenegger (1) Harald Rennhofer (1) Charbel Sakr (1) Thomas Srdinko (2) Christina Streli (2)

(1) Universität für Bodenkultur Wien (BOKU)
(2) TU Wien

Mechanical properties of biological materials are strongly dependent on the nano- and microstructure of the materials. By measuring the orientation of fibers or nanocrystallites it is possible to gain insight into their physical properties. Standard X-ray diffraction is a well-established technique for this kind of measurements but needs multiple measurements involving sample rotation to reconstruct the fiber orientation, which is often not easily doable for biological samples due to their complex morphology.
We present an alternative approach, where crystallographic texture information can be obtained in a single measurement, called Energy Dispersive Laue Diffraction (EDLD). The newly set-up X-ray Color Camera Microscope hosts a modern, pixelated CCD-based X-ray detector, and can provide direct detection of X-rays with both energy and spatial resolution. Using a broad spectrum of photon energy, sample rotation is not needed to provide three-dimensional information in a single shot. We will show measurements on different biological materials from the synchrotron as well as from the lab setup, using a modern high-flux lab source.

M34 – Session 2 (Tue 22, 16:00-18:00, Chair: Oskar Paris)

ID	Title	Speaker	Type
138	**Nature's Blueprint: Water-Enabled Functionalities in Hierarchically Porous Solids**	Patrick Huber	Invited talk (16:00-16:30)

Patrick Huber (1,2)

(1) Hamburg University of Technology
(2) Deutsches Elektronen-Synchrotron DESY

The exquisite diversity and functionality of biological materials is truly remarkable, especially since they are composed of a small set of abundant chemical elements. While engineering materials primarily require specific, often unsustainable, chemical compositions to realize their functions, nature achieves unparalleled functionality through optimized architectures that span multiple length scales. Water, with its ubiquity and unique structural dynamics, plays a pivotal role as a nanoscale "working fluid" in shaping the properties and functionality of nature's materials. Here, I will introduce a novel class of sustainable, interactive materials that derive their functionality from the interplay between hierarchical structures of hard matter and water as a soft actor. I will show how these "Blue Materials " can mimic natural processes such as water-driven mechanical actuation, capillarity-driven water transport, and humidity-responsive coloration and light scattering. I will also highlight their potential for innovative applications, including electrical energy storage and energy harvesting from low-grade waste heat, thus extending the functionalities observed in nature.

134	**Probing Interfacial Structure and Collective Dynamics under Applied Potential with THz Spectroscopy**	Nina Strasser	Contributed talk (16:30-16:45)

Nina Strasser (1) Nicolai Wichmann (1) Jaspreet Kaur (1) Melinda Nolten (1) Mohammed Jassar (2) Qiwei Yao (2) Taline Kerackian (3) Simone Pezzotti (2) Gerhard Schwaab (1) Siegfried Waldvogel (3) Martina Havenith (1)

(1) Ruhr-University Bochum
(2) Ecole Normale Supérieure de Paris
(3) Max Planck Institute for Chemical Energy Conversion

Understanding aqueous interfaces at electrified metal surfaces remains a fundamental challenge, as continuum descriptions treat the solvent as a homogeneous medium and thus neglect its molecular nature. In particular, the neglect of hydrogen bonding and density fluctuations highlights the need to go beyond classical mean-field approaches.
A striking example of this breakdown is provided by molecular dynamics simulations at constant applied potential at the gold-water interface, representing a prototypical “soft meets hard” system. [1] While the first interfacial water layer forms a highly ordered, two-dimensional hydrogen-bond network, the adjacent layer exhibits markedly reduced connectivity. This leads to a situation where water effectively “repels” water, resulting in the formation of cavities at the interface that preferentially host small molecules such as CO or N_2.
To experimentally probe such effects, we employ terahertz (THz) spectroscopy under externally controlled electric fields, providing direct access to collective intermolecular vibrations at charged interfaces. [2] To the best of our knowledge, this represents the first setup capable of probing such dynamics

under an applied potential. As an initial application, this setup enables the direct observation of a hydrophobic cation-rich film, which profoundly reshapes the electric double layer. [3]
Building on this approach, we extend our investigation to different tetraalkylammonium-based species and aqueous electrolytes. By systematically varying the cation hydrophobicity and tuning the anion size, we reveal how ion-specific interactions drive the formation of interfacial films. We further combine THz spectra with molecular dynamics simulations to gain molecular-level insight into the underlying mechanisms.

[1] A. Serva, et al., PNAS, 118, e2023867118 (2021).
[2] S.R. Alfarano, et al., PNAS 118, e2108568118 (2021).
[3] N.S. Wichmann, et al., JACS, 148, 13, 13550-13560 (2026).

183	**How Do Aqueous Supercapacitors Capture CO_2? Establishing a Mechanistic Understanding**	Malina Seyffertitz	Contributed talk (16:45-17:00)

Malina Seyffertitz (1) Jack S. Taylor (1) Zeke Coady (1) Cerys Walsh (1) Alexander C. Forse (1)

(1) University of Cambridge

Supercapacitors are a perfect example of a soft meets hard interface: they consist of two nanoporous electrodes submerged in a liquid electrolyte. When a voltage is applied across the electrodes, the ions in the electrolyte move accordingly and form electric double layers at the electrode-electrolyte interfaces to balance the charge. This interfacial charge separation enables rapid, reversible charge storage through dominantly electrostatic (non-faradaic) processes, thereby supporting high power density and long cycle life. Accordingly, supercapacitors are widely used for high power energy storage applications. More recently, however, it has been discovered that exposing one supercapacitor electrode to a CO2 containing gas also enables reversible and largely selective CO2 capture upon charging, known as Supercapacitive Swing Adsorption (SSA) [1].
This electrochemical CO2 capture approach inherits several attractive features from supercapacitors, including long cycle lifetimes, inherent tolerance to humidity in the gas stream, the use of abundant and sustainable materials, and low energy consumption without the need for thermal regeneration. However, despite growing interest and extensive empirical optimisation, the fundamental mechanism governing CO2 adsorption and desorption in supercapacitors has remained unresolved.
Here, we identify the mechanism of CO2 capture in aqueous supercapacitors, showing that it is governed by an electrochemical pH swing at the electrode-electrolyte interface. This pH swing modulates carbon speciation and the dissolved inorganic carbon content in the electrolyte, driving CO2 uptake and release from the gas phase. Using operando monitoring in a dedicated supercapacitor setup for SSA, we quantify local pH changes during charging and discharging. Negative electrode polarisation induces more basic conditions, driving CO2 uptake, while positive polarisation leads to local acidification and consequently CO2 release. Calculated changes in dissolved inorganic carbon as a function of pH are in excellent quantitative agreement with experimentally measured CO2 uptake and release. Furthermore, suppressing pH changes using a buffered electrolyte almost completely suppresses CO2 capture, confirming that pH is the controlling variable.
By identifying local pH changes as the governing factor for CO2 capture and release in supercapacitors, this work resolves the long-standing lack of mechanistic understanding in SSA and provides a first foundation for controlling and improving performance in supercapacitor-based electrochemical CO2 capture systems.

[1] B. Kokoszka, N. K. Jarrah, C. Liu, D. T. Moore and K. Landskron, Angew. Chem. Int. Ed., 2014, 53, 3698–3701

416	**Operando Synchrotron Analysis of Capacitive Water Desalination Electrodes**	Max Rauscher	Contributed talk (17:00-17:15)

Max Rauscher (1) Sylvio Haas (2) Richard Kohns (3) Johannes Liebhart (1) Oskar Paris (1) Malina Seyffertitz (4)

(1) Montanuniversität Leoben, Lehrstuhl für Physik
(2) Centre for X-ray and Nano Science CXNS, Deutsches Elektronen-Synchrotron DESY, 22607 Hamburg, Germany
(3) Institute for Materials and X-Ray Physics, Hamburg University of Technology, 21073 Hamburg, Germany
(4) University of Cambridge

Understanding ion storage and transport in nanoporous electrodes for water desalination requires sophisticated experimental methods that can resolve how and in which pore regime ion concentration changes occur during operation. This information can be provided by operando X-ray techniques. Here, we present a correlative synchrotron approach under realistic operating conditions. We obtain element specificity with pore-hierarchy sensitivity within an electrochemical cell during charging and discharging by combining position- and time-resolved X-ray fluorescence (XRF), X-ray transmission (XRT), and Small-Angle X-Ray Scattering (SAXS).
We report an operando SAXS, XRF, and XRT study of electrochemical cells with 50 mM RbBr and $SrBr_2$ aqueous electrolytes. Carbon electrodes with hexagonally organized mesopores and disordered micro- and macropores serve as a hierarchically porous model system. Separating distinctive diffraction peaks from the ordered mesopores and the diffuse scattering from macro- and mesopores allows quantifying variations in electron density across several pore regimes of the hierarchical electrodes with SAXS. While XRF maps Rb, Sr, and Br to offer ion-specific concentration information, XRT reports the average concentration change within the electrodes.
Together, these methods offer cross-validation and reduce uncertainty in the interpretation of each individual signal, creating a cohesive picture of the relationship between changes in total concentration, ion species, and pore-scale specific response. In this way, the correlative synchrotron radiation approach allows to uniquely determine local charge balancing mechanisms, and helps understanding dynamic effects related to ion transport and accessibility in hierarchical electrode materials.

341	**Interactions At Carbon–Electrolyte Interfaces In Aqueous Organic Redox Flow Batteries**	Ahmad Alem	Contributed talk (17:15-17:30)

Ahmad Alem (1) Christine Bandl (1) Michael Feuchter (1) Johannes Liebhart (1) Bernhard Marius (2) Oskar Paris (1) Christoph Rameshan (1) Max Rauscher (1) Alexa Scheer (3) Stefan Spirk (3) Matheus A. Tunes (1) Nicole Wechner (1) Dominik Wickenhauser (2)

(1) Technical University of Leoben, Leoben, Austria
(2) Ecolyte GmbH, Graz, Austria
(3) Graz University of Technology, Graz, Austria

Interfaces between aqueous electrolyte and porous carbon electrodes critically govern the performance of organic redox flow batteries (ORFBs). In this work, we investigate how pretreatment strategies including O2 plasma, KOH activation, and CO2 activation modify the interfacial properties of carbon felt

electrodes by tuning surface chemistry, defect structure, and porosity. Using X-ray photoelectron spectroscopy (XPS), Raman spectroscopy, scanning electron microscopy (SEM), and inverse gas chromatography (iGC), we establish a structure–property relationship linking these modifications to electrochemical behavior in an quinone-based aqueous electrolyte. Although all treatments reduced activation losses, only CO2-activated electrodes maintained enhanced performance over extended cycling (up to 280 cycles). This enhanced performance correlates with the significantly increased surface area and higher defect density introduced by CO2 activation, which promote improved interfacial accessibility and electrochemical activity. While surface fouling that blocks active sites is observed for all samples, CO2-activated electrodes retain superior activity, indicating that interfacial transport and accessibility, rather than surface chemistry alone, govern long-term performance. These results demonstrate that different pretreatment pathways selectively control key aspects of interfacial interactions, including chemical functionality, defect-driven reactivity, and pore structure. This provides design guidelines for developing durable, high-performance electrodes in ORFB systems.

M35 - Lipids, Surfactants and Polyelectrolytes

M35 – Session 1 (Mon 21, 16:00-18:00)			
ID	Title	Speaker	Type
803	**Studying the in-plane structure of non-crystalline lipid layers with X-ray scattering techniques and molecular simulations**	Emanuel Schneck	Invited talk (16:00-16:30)

Emanuel Schneck (1)

(1) TU Darmstadt, Department of Physics, Darmstadt, Germany

804	**Disorder to Order: Streamlining Biomolecule Simulation Re-Use with FAIR NMRlipids database**	Markus Miettinen	Invited talk (16:30-17:00)

Markus Miettinen (1)

(1) Department of Chemistry, University of Bergen, Norway

277	**2D Network of PDMS and PEO-PPO-PEO at the air-water interface**	Ellen Backus	Contributed talk (17:00-17:15)

Ellen Backus (1) Aurély Araminthe (2) Sophie Cantin (2) Alae El Haitami (2) Bence Kővágó (1)

(1) Universität Wien
(2) CY Cergy Paris Université

Thin polymer films based on polymer blends can be used as coatings with tunable properties. Such films can be created with the Langmuir film method: polymers are deposited on water controlling their density by compression, potentially cross-linked to obtain networks, and subsequently transferred onto a solid substrate resulting in stable thin films. As a first step to design such films, the miscibility properties of non-cross-linked polymer blends must be understood. In this work, we focus on understanding the miscibility properties of amphiphilic poly(ethylene oxide)-poly(propylene oxide)-poly(ethylene oxide) (PEO-PPO-PEO) triblock copolymer and predominantly hydrophobic poly(dimethylsiloxane) (PDMS). We analyzed surface pressure-area isotherms to determine the phase transitions of the blends and used Brewster angle microscopy (BAM) to understand the mixing behavior at the interface. We combined these results to build a surface pressure-composition phase diagram and identified a miscibility region independent of composition at low surface pressure. To connect the phase diagram with molecular level information, sum frequency generation (SFG) spectroscopy has been performed. With this method basically the vibrational spectrum of the interface can be obtained. From peak amplitudes in the CH-OH and CO spectral region, we conclude that polymers change their orientation after the phase transition. To make a stable network, as a second step towards coatings, light induced cross linking of the end groups of the PDMS in the miscibility region on the water surface has successfully been conducted.

802	**NLP toxins form transient pores in plant cell membranes**	Jure Derganc	Contributed talk (17:15-17:30)

Jure Derganc (1) Nika Zibrat (2) Mojca Mally (1) Gregor Anderluh (2)

(1) Institute of Biophysics, Faculty of Medicine, University of Ljubljana, 1000 Ljubljana, Slovenia
(2) Department of Molecular Biology and Nanobiotechnology, National Institute of Chemistry; 1000 Ljubljana, Slovenia

Necrosis- and ethylene-inducing peptide 1-like proteins (NLPs) are a large family of microbial toxins secreted by taxonomically diverse pathogens—including bacteria, fungi, and oomycetes—that infect a wide range of crops such as potato, tomato, soybean, and grapevine. These pathogens significantly burden global agriculture. A sad example is Phytophthora infestans, an NLP-producing oomycete that caused the Great Irish Famine. NLPs interacts with plant membranes through glycosylinositol phosphorylceramides (GIPCs), but the specificity of these interactions and the mechanism of toxicity remain unclear. We used microfluidic assays on giant unilamellar vesicles (GUVs) to study NLP binding and pore formation in GIPC-containing membranes (Pirc et al., 2022; Žibrat et al., 2025). Binding of diverse cytotoxic NLPs was observed on membranes containing GIPCs from monocots or dicots, but not on control POPC membranes with or without sterols. The microfluidic setup allowed precise monitoring of binding dynamics and subsequent vesicle leakage, revealing a time lag between NLP binding and leakage. Corroborated by other approaches—including conductance measurements across planar lipid bilayers, high-speed AFM, and MD simulations—these results show that NLPs form transient pores without penetrating the membrane, which is in stark contrast to pore-forming toxins such as lysenin.

Pirc et al. (2022). An oomycete NLP cytolysin forms transient small pores in lipid membranes. Science Advances, 8(10), eabj9406.
Žibrat Kalanj et al. (2025). Surface plasticity of the cytotoxic Nep1-like protein enables promiscuity in binding to its lipid receptor glycosylinositol phosphorylceramides. Science Advances, 11(41), eadw6401.

564	**Rhamnolipid Segregation in Mixed Monolayer Membranes Probed by Contrast-Variation SANS**	Florian Trummer	Contributed talk (17:30-17:45)

Florian Trummer (1) Raj Kumar (2) Rika Raff (1) Thomas Sottmann (1)

(1) Universität Stuttgart, Institut für Physikalische Chemie
(2) University of Strathclyde, Department of Pure and Applied Chemistry

In recent years, biosurfactants have been sparking increasing interest in both, academic research and industry, as an alternative to conventional, petrochemical-derived surfactants. From an application point of view, the use of biosurfactants allows for more biocompatible formulations that are also

less harmful to the environment, due to a lower CO_2 footprint in production and their enhanced biodegradability. Their aggregation behaviour and interfacial activity in solution, however, is far from being fully understood and often depends on a multitude of parameters, e.g. pH, ion concentration or temperature. Rhamnolipids, a class of glycolipids that is produced by microorganisms, are among the most thoroughly researched biosurfactants [1,2]. In our current research, we are focussing on biocompatible microemulsion formulations, which are an interesting basis for, e.g. cosmetic or detergent applications due to their ultralow interfacial tension between water and oil phases and excellent wetting properties. in the quaternary system H_2O – Isopropylmyristate (IPM) – di-Rhamnolipid ($Rha_2C_{10}C_{10}$) – Octane-1,2-diol, where IPM is used as nonpolar oil phase, while Rha2C10C10 and octanediol serve as surfactant and hydrophobic co-surfactant respectively. The use of a co-surfactant allows to tune the composition of the interfacial film, which is a key parameter to influence its curvature, allowing to drive a system through phase inversion from oil-in-water to water-in-oil microemulsions via the balanced, bicontinuous morphology [3].
Having extensively studied the phase behaviour of these quaternary microemulsions, we recently had the opportunity to carry out contrast variation SANS experiments with the goal to investigate the composition of the interfacial film at different temperatures. To this end, we first used deuterated IPM to reach film contrast conditions (i.e. a contrast matching of the aqueous and oil phase) and subsequently d-octanediol to reach a rhamnolipid contrast (matching of the aqueous, oil, and octanediol components). To our surprise, we found an untypical scattering behaviour at high q, pointing towards an uneven distribution of $Rha_2C_{10}C_{10}$ molecules in the amphiphilic film or a very defined conformation of the rhamnolipid's double sugar head group. Our results highlight the power of contrast variation SANS in the study of novel surfactants and how it needs to be coupled with other studies, such as molecular dynamics or high-resolution NMR to understand the complex interfacial aggregation behaviour of this important class of biosurfactants.

[1] N. Baccile et al. Langmuir 2023, 39 (27), 9273-9289.
[2] P. Le Bastart de Villeneuve, F. Trummer et al. J. Mol. Liq. 2025, 436, 128271.
[3] R. Strey, M. Jonströmer J. Phys. Chem. 1992, 96(11), 4537-4542.

704	**Influence of headgroup chemistry and sterols on in-plane structural correlations of fluid lipid monolayers**	Konrad Weber	Contributed talk (17:45-18:00)

Konrad Weber (1)

(1) TU Darmstadt, Department of Physics, Darmstadt, Germany

Fluid lipid monolayers at the air/water interface provide a uniquely controllable model system for probing the molecular interactions that govern biological membrane organization. In cellular membranes, the chemical identity of lipid headgroups and the presence of sterols such as cholesterol critically shape lateral packing, domain formation, and the dynamic balance between order and fluidity. Yet, despite their central biological relevance, the in-plane structural correlations within the liquid-expanded (LE) phase remain comparatively underexplored. Using state-of-the-art X-ray diffraction (GIXD), it is possible to investigate how headgroup chemistry and sterol incorporation influence the short-range structural correlations of such fluid monolayers. The systematic comparison of monolayers containing different phospholipids and glycolipids, as well as varying molar ratios of phosphatidylcholines and cholesterol reveal how the organization of their in-plane structure is either enhanced or disrupted depending on the lipid environment.

M35 – Poster session (PS1 Mon21-Tue22)

ID	Title	Presenter	Type
190 **P025**	**Coupling of membrane asymmetry to the function of an integral membrane enzyme**	Shalini Mishra	Poster

Shalini Mishra (1) Shahrzad Dabironezare (1) Niclas Decker (1) Michael Kaltenegger (1) Georg Krainer (1) Georg Pabst (1)

(1) University of Graz

Plasma membranes are intrinsically asymmetric, with the two leaflets differing in lipid composition. This compositional asymmetry alters lateral pressure profiles, curvature, and hydrophobic thickness, which can modulate the function of embedded membrane proteins. To elucidate how membrane asymmetry couples to membrane protein function, our lab reconstitutes proteins into compositionally well-defined mimics of plasma membranes. We focus on the outer membrane phospholipase A (OmpLA), an integral membrane lipase from the outer membrane of Gram-negative bacteria. Asymmetric large unilamellar proteoliposomes (aPLUVs; size: ~ 100 nm) containing OmpLA were generated via cyclodextrin-mediated lipid exchange using mixtures of monounsaturated phosphatidylethanolamine, phosphatidylcholine, phosphatidylglycerol and phosphatidylserine. Membrane structure and thermotropic behavior were characterized by combined small-angle X-ray and neutron scattering, together with differential scanning calorimetry. To probe the functional consequences of asymmetry, we monitored OmpLA dimerization in asymmetric bilayers as a readout of its enzymatic activation. For this, we employed an inactive OmpLA variant site-specifically labeled with AF488 or AF647 to enable Förster resonance energy transfer (FRET), and performed single-molecule FRET measurements on a custom-built confocal microscope. Our results provide first insights into how lipid bilayer asymmetry modulates OmpLA dimerization and activity, highlighting a direct link between the asymmetric physical properties of the membrane and the functional state of an integral membrane enzyme.

196 **P026**	**Effect of an Integral Membrane Enzyme on the Structure of Asymmetric Lipid Bilayers**	Shahrzad Dabironezare	Poster

Shahrzad Dabironezare (1) Jackson Crowley (2) Niclas Decker (1) Sara Eckhardt (3) Daniel Huster (3) Shalini Mishra (1) Georg Pabst (1) Lionel Porcar (4) Enrico Semeraro (1) Robert Vácha (2)

(1) University of Graz
(2) CEITEC Masaryk University
(3) Leipzig University Germany
(4) Institut Laue Langevin

All biological plasma membranes are intrinsically asymmetric in their lipid composition across the two leaflets, a feature believed to be essential for maintaining membrane integrity and enabling efficient cellular signaling [1].

In this work, joint small-angle X-ray and neutron scattering (SAXS/SANS) experiments are used to resolve leaflet-specific structural properties of 100 nm large unilamellar vesicles and proteoliposomes. Specifically, we are focusing on the outer membrane phospholipase A (OmpLA) from Gram-negative bacteria as a prototypical β-barrel integral protein and its effect on asymmetric lipid bilayers. Both symmetric and asymmetric membranes are prepared with and without reconstituted OmpLA across a range of lipid compositions and protein concentrations using established protocols [2].
To resolve the individual membrane leaflets we apply contrast variation in SANS experiments using chain deuterated lipids and different D_2O/H_2O ratios. We provide first insights from a newly developed analysis platform SAS-MoCa which applies Bayesian inference to combine the SAXS/SANS data with complementary molecular dynamics simulations and H-NMR experiments.

[1] Schütz, G. J., Pabst, G. (2023). The asymmetric plasma membrane—A composite material combining different functionalities? BioEssays, 45, e2300116.
[2] Doktorova, M., Heberle, F.A., Eicher, B. et al. (2018) Preparation of asymmetric phospholipid vesicles for use as cell membrane models. Nat Protoc 13, 2086–2101.

274 **P027**	**Surfactant Adsorption at Interface: An Atomistic Free Energy Approach**	Vid Pograjc	Poster

Vid Pograjc (1) Matej Kanduč (1)

(1) Jožef Stefan Institute

Surfactants are amphiphilic molecules that spontaneously adsorb and self-organize at aqueous interfaces, a process central to numerous technological and biological applications ranging from detergency and emulsification to drug delivery and foam stabilization. Their interfacial behavior is governed by the balance between hydrophilic and hydrophobic interactions, which also determines the timescale on which individual molecules exchange between the interface and the bulk solution. The exchange time grows exponentially with alkyl chain length, increasing by a factor of 2–3 per CH_2 group, spanning many orders of magnitude across different surfactant classes.
Short-chain surfactants (≤C8) exchange on nanosecond timescales, allowing adsorption equilibria to be directly monitored in all-atom MD simulations. For intermediate-chain surfactants (C9–C18), which constitute the most industrially prevalent class, exchange times range from microseconds to seconds, far beyond what atomistic MD can directly access, creating a fundamental gap between simulation capabilities and the most practically relevant surfactants.
To overcome this, we employ a molecular thermodynamic theory (MTT) framework enforcing equal chemical potentials across coexisting phases. As input, transfer free energies — defined as the free energy cost of moving a surfactant molecule from the interface into bulk water — are computed via thermodynamic integration in all-atom MD simulations, from which adsorption and pressure isotherms are derived. The approach is validated using a C6 surfactant, for which adsorption is computed both from direct equilibrium MD simulations and from the MTT framework.

317 **P028**	**Probing hydrophobic mismatch-mediated protein-protein interactions by single-molecule FRET**	Michael Kaltenegger	Poster

Michael Kaltenegger (1) Georg Krainer (1) Shalini Mishra (1) Georg Pabst (1)

(1) University of Graz

Cellular membranes are highly complex composite materials composed of lipids and proteins. The diverse physiological functions of these membranes, such as transport of molecules or signaling are controlled by intricate interactions between lipids and proteins across molecular to mesoscopic length scales. Among these, interactions due to a mismatch between the hydrophobic length of integral membrane proteins and the hydrophobic thickness of their hosting lipid bilayers may modulate protein conformational equilibrium and thereby influence their function.
In this project, we used the well-examined outer membrane phospholipase A (OmpLA) to observe the impact of hydrophobic mismatch on protein-protein interactions at the single molecule level. OmpLA hydrolyses phospholipids upon the formation of homodimers. We thus reconstituted a fluorescently labeled and inactive variant of OmpLA into lipid vesicles to probe its dimerization equilibrium as proxy for its activity. Specifically, we used single molecule Förster resonance energy transfer (smFRET) on a custom-built single molecule confocal microscope, which allowed to simultaneously keep track of the interprotein distance and the stoichiometry of FRET pairs. Control experiments of OmpLA dimerization were performed in zwitterionic micelles. By systematically varying lipid composition, we explored conditions of positive and negative hydrophobic mismatch and identified distinct effects on OmpLA dimerization behaviour. Our results demonstrate how bulk membrane properties can regulate the interactions and functional states of integral membrane proteins, providing insights into the physical mechanisms underlying the coupling of bulk membrane properties and integral membrane proteins.

521 **P029**	**Surfactant adsorption at the contact line of water nanodroplets**	Fabio Staniscia	Poster

Matej Kanduč (1) Fabio Staniscia (1)

(1) Jožef Stefan Institute

We investigate the adsorption of surfactants in sessile water nanodroplets on solid hydrophobic substrates. Using molecular dynamics simulations, we provide evidence that surfactants, which in our case are linear alcohols or aromatic molecules, show an excess of adsorption close to the three-phase contact line. This result reveals that surfactants have a higher affinity for the contact line than for the water-vapor and water-substrate interfaces.
We characterize this phenomenon by investigating the surface and line adsorption isotherms of the different species and show that, at small concentrations, they follow a qualitatively similar behavior. This allows us to extract the coefficients quantifying their affinity for the two interfaces and for the contact line, and derive general rules describing their dependence on the chemical characteristics. In particular, for linear surfactants, we find an exponential dependence on the number of carbon atoms.
At higher concentrations, the behavior of surfactants starts differentiating, and the adsorption isotherms exhibit a rich phenomenology, characterized by a complex dependence of the partitioning between the different regions of the droplets (bulk, interfaces, and contact line) on concentration.
We then investigate the dependence of the partitioning on droplet size, and calculate the influence of line adsorption on line tension, showing that it has the effect of reducing it, in a similar fashion as surface adsorption does with surface tension. We finally investigate the implications of this effect on the determination of contact angles.

724 **P030**	**Ion-tunable DNA Oligo-Catenanes with Mechanical Heterogeneity**	Terpsichori Alexiou	Poster

Terpsichori Alexiou (1) Christos Likos (1)

(1) Faculty of Physics, University of Vienna

Atomistic molecular dynamics simulations are conducted on aqueous ionic solutions containing catenated pairs of double-stranded DNA (dsDNA) minicircles [1-3] that feature flexible single-stranded (ssDNA) segments along their contour. Effective pair interaction potentials are evaluated as functions of the center-of-mass separation between the heterogeneous minicircles. The effects of ion type, ionic strength, and ssDNA segment length on the resulting effective interactions are systematically analyzed. The results provide fundamental insight into how localized flexibility modulates the structural dynamics, rotational behavior, and emergent functionalities of DNA-based nanostructures.

(1) Alexiou, T. S.; Alatas, P. V.; Tsalikis, D. G.; Mavrantzas, V. G. Conformational and Dynamic Properties of Short DNA Minicircles in Aqueous Solution from Atomistic Molecular Dynamics Simulations. Macromolecules 2020, 53 (14).
(2) Alexiou, T. S.; Likos, C. N. Effective Interactions between Double-Stranded DNA Molecules in Aqueous Electrolyte Solutions: Effects of Molecular Architecture and Counterion Valency. Journal of Physical Chemistry B 2023, 127 (31).
(3) Alexiou, T. S.; Likos, C. N. Ion-Specific Modulation of the Conformation and Compactness of DNA Oligo-Catenanes. Journal of Physical Chemistry B 2026, 130 (2).

M36 - Physics of Cellulose-based Materials

M36 – Session 1 (Fri 25, 10:30-12:45, Chairs: Karin Zojer, Eduardo Machado, Robert Schennach)			
ID	Title	Speaker	Type
144	**Unraveling Overlapping Sorption and Release Dynamics in Paper: A Multi-Process Kinetic Perspective**	Alexandra Serebrennikova	Invited talk (10:30-11:00)

Alexandra Serebrennikova (1) Raimund Teubler (2) Karin Zojer (3)

(1) Wood K plus, Competence Centre for Wood Composites and Wood Chemistry
(2) Institute of Analytical Chemistry and Food Chemistry, Graz University of Technology
(3) Institute of Solid State Physics, Graz University of Technology

The interaction of volatile molecules with paper as a complex porous material is governed by coupled transport and sorption processes that are often experimentally indistinguishable when only overall uptake dynamics are considered. In this contribution, we present a strategy to resolve such overlapping processes using the model system of dimethyl sulfoxide (DMSO) vapor interacting with cellulose-based paper. While conventional sorption curves suggest a single effective process, we demonstrate that the release dynamics reveal the presence of at least two distinct molecular populations characterized by markedly different kinetic time scales.
By combining time-resolved uptake measurements with controlled partial desorption experiments, we separate the contributions of a rapidly exchanging population and a strongly retained population. These exhibit characteristic release rates differing by several orders of magnitude (~10^{-4} s^{-1} vs. ~10^{-6} s^{-1}), enabling the reconstruction of individual sorption kinetics for each population. This approach allows us to extract process-specific rate constants and activation energies, providing insight into the underlying physical mechanisms.
We interpret the fast population as weakly bound molecules associated with surface interactions and evolving fiber morphology, while the slow population is attributed to molecules trapped within the fiber wall. The results highlight that apparent single-process behavior can mask fundamentally different transport and interaction regimes in porous media. More broadly, the methodology offers a general framework for disentangling simultaneous kinetic processes in complex materials where standard approaches fail.
This work advances the understanding of mass transport in paper and related porous systems, with implications for applications ranging from barrier materials and packaging to functional cellulose-based materials.

419	**Influence of Alkali Counterions on the Refractive Index of Sulfated Cellulose Nanocrystals**	Maximilian Fuchs	Contributed talk (11:00-11:15)

Maximilian Fuchs (1) Ali Khodayari (2) Daniel Knez (3) Tiina Nypelö (Department of Bioproducts and Biosystems, Aalto University, Espoo, Finland) David Seveno (2) Stefan Spirk (1) Wim Thielemans (4) Agnes Weiß (1)

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(2) Department of Materials Engineering, KU Leuven, Kasteelpark Arenberg 44, 3001, Leuven, Belgium
(3) Institute of Electron Microscopy and Nanoanalysis, NAWI Graz, Graz University of Technology, Steyrergasse 17, Graz 8010, Austria
(4) Sustainable Materials Lab, Department of Chemical Engineering, KU Leuven, Campus Kulak Kortrijk, Etienne Sabbelaan 53, 8500, Kortrijk, Belgium

Cellulose nanocrystals (CNCs) are rod-like, highly crystalline nanoparticles. They are derived from cellulose, the most abundant biopolymer on Earth. Despite extensive work on CNCs, their refractive index (RI) is still not conclusively established. Reported values vary depending on the sample state and measurement method [1,2]. For sulfated CNCs, counterions are likely responsible for some of these variations. Counterions are bound to the sulfate half-ester groups and may modify the hydration environment at the CNC surface [6]. Understanding these interactions is relevant not only for RI measurements but also for fundamental CNC studies. Alkali ions can serve as labels in ultrastructural investigations, as we previously demonstrated [5].
This study examines how different alkali metal ions (from Li^+ to Cs^+, including H^+) as counterions on the CNC surface affect the apparent refractive index. To assess whether sample preparation contributes to the measured RI, several exchange procedures are compared. These include a dialysis-based route and two different cation-exchange resins [4]. For all procedures, pH is adjusted to 7, and ultrasonication is applied to reduce agglomeration, as this step highly influences the measured RI.
Two optical methods are used. In the first, an established dispersion-based approach measures CNC suspensions by refractometry at different concentrations. The data are then extrapolated to obtain an effective RI of the CNC in water [1,2]. In the second method, spin-coated CNC thin films are analyzed by surface plasmon resonance (SPR) in air and isopropanol. Unlike refractometry, SPR probes a substantially less hydrated state. A cellulosic layer was also probed as a binding layer between the gold substrate and the CNCs. This additional RI data on pure cellulose shows that CNCs have a lower RI than pure cellulose, as previously reported [3]. Our results further show that heavier alkalis, such as Cs-CNCs, exhibit a lower RI than H-CNCs and lighter alkali forms. Although the absolute RI values differ between refractometry and SPR, both methods show a comparable decrease of about 0.03 in the RI from H-CNCs to Cs-CNCs. In SPR, this relative difference appears at all three investigated wavelengths. Overall, these findings indicate that the absolute RI depends on the measurement environment, while the relative counterion effect appears robust in the dataset. The different patches and exchange procedures only show minor variations in both measurement methods.

[1] Landry et al., For. Prod. J. 2011, 61, 104–112.
[2] Saveyn et al., Part. Part. Syst. Charact. 2002, 19, 426–432.
[3] Reid et al., Langmuir 2017, 33, 7403–7411.
[4] Petschacher et al., Nanomaterials 2022, 12, 3131.
[5] Knez et al., Small 2025, 21, 2500351.
[6] Ikegami, J. Polym. Sci. A-2 1964, 2, 907–921.

532	**Combined modelling and scattering studies on cellulose microfibril structures and their water interactions**	Antti Paajanen	Invited talk (11:15-11:45)

Antti Paajanen (1) Aleksi Zitting (2) Jukka Ketoja (1) Tuukka Verho (1) Paavo Penttilä (3)

(1) VTT Technical Research Centre of Finland Ltd
(2) Aalto University
(3) University of Jyväskylä

Progress in understanding the molecular architecture of wood secondary cell walls has enabled the use of computational methods, and molecular simulation in particular, to investigate their nanostructure and water interactions. We report simulation studies that address the structure of wood cell walls, and cellulosic materials derived from them, at different length scales and levels of approximation. We develop molecular models of cellulose microfibrils both as individual nano-objects and in aggregated states mimicking their cell wall environment, considering also their interactions with hemicelluloses, lignin and water. We carry out simulations of their response to drying and compare the predictions, among others, to X-ray and neutron scattering experiments on Norway spruce wood samples. The models reproduce detailed features of the experimental data, thus supporting the underlying structural hypotheses. Our findings provide insight into the structure and stability of microfibril interfaces, their role in stress transfer and in controlling water diffusivity. We further develop stochastic three-phase models of aligned microfibril structures in the sub-100 nm length scale, and use them as a basis for a scattering analysis tool for wood samples. Besides contributing to the understanding of wood cell wall nanostructure, our research addresses phenomena that are relevant for many of the current processing routes and uses of cellulosic raw materials.

778	**Fibre Geometry Shapes Pore Architecture: Micro-CT and SNOW-Based Analysis of Cellulose Absorbent Materials**	Thomas Harter	Contributed talk (11:45-12:00)

T. Harter (1,2) M. Fuchs (3,4) E. Machado Charry (3) I. Bernt (2,5) E. Baikova (3, 4) A. Maaß (1,2) R. Schennach (3) K Zojer (3, 4) U. Hirn (1,2)

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(3) Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz
(4) CD Laboratory for mass transport through paper, Petersgasse 16, 8010 Graz, Austria
(5) Kelheim Fibres GmbH, Regensburger Straße 109, Kelheim, Germany

Porous cellulose networks form the structural backbone of absorbent hygiene materials, where internal pore architecture directly governs fluid retention capacity. Despite this, engineering-focused investigation of tampon pore structure remains scarce. This study applies micro-computed tomography (micro-CT) combined with the sub-network of an over-segmented watershed (SNOW) algorithm and PoreSpy to characterize the three-dimensional pore structure of tampon proxy materials made from round and trilobal cellulose viscose fibres after liquid absorption. Otsu segmentation was used to binarize the reconstructed volumes, and pore size distributions were extracted as pore equivalent diameters (PED) across four spatial positions per sample.
Trilobal fibre proxies exhibited consistently larger pores than their round-fibre counterparts, with median PED values 26–32% higher across all measurement positions, despite comparable bulk porosity (~82–85%). This finding highlights that bulk porosity alone is insufficient to characterize absorbent performance, and that pore size, shaped by fibre cross-sectional geometry, is the more discriminating parameter. The higher surface area and longitudinal channel structures of trilobal fibres promote more extensive network expansion upon liquid uptake, yielding a more open pore architecture and 18.7% greater absorbency. Kolmogorov-Smirnov distance analyses confirm that inter-fibre differences in pore structure substantially exceed intra-sample positional variations, underscoring the dominant influence of fibre geometry over production-induced gradients. A systematic top-to-bottom decrease in pore size was also observed, likely reflecting one-sided liquid application and compression effects during manufacturing. These results establish micro-CT combined with SNOW-based void space partitioning as an effective methodology for characterizing pore networks in fibrous cellulose materials and provide a mechanistic basis for optimizing absorbent product design.

689	**A rate-dependent finite-strain model of flax fibres with plasticity-induced evolution of orthotropy**	Manfred H. Ulz	Invited talk (12:00-12:30)

Manfred H. Ulz (1) Caterina Czibula (2) Christian C. Celigoj (1)

(1) Graz University of Technology
(2) Northwestern University

Flax fibres have attracted increasing interest in recent years, with growing applications in non-wovens, fibre-reinforced composites and other bio-based materials. They exhibit significant variability in geometry, microstructure and defect content, which in turn affects their mechanical response. At the level of a single fibre, this results in a hierarchically organised material system whose effective behaviour is governed by its multi-scale internal structure and can be described, from a continuum-mechanical perspective, as a transversely isotropic material.
In this study, cyclic tensile experiments were conducted on individual flax fibres. The measured stress-strain response was analysed for several loading rates in order to characterise rate-dependent effects, hysteresis, plastic strain and changes in stiffness during repeated loading and unloading. The experimental observations of these features provide the target behaviour for the development of a constitutive model.
The formulation of a finite-strain constitutive framework for the rate-dependent response of flax fibres is presented. The model extends a rate-independent formulation previously developed, which combined orthotropic elasticity and orthotropic plasticity in a covariant hyper-elasto-plastic setting. In this approach, plastic deformation induces an evolution of the orthotropic material directions, thereby describing deformation-induced changes in material symmetry. This mechanism is conceptually related to the notion of plastic spin and enables the model to reproduce the experimentally observed increase in stiffness. The present contribution extends the framework by incorporating viscous effects in both the elastic and plastic parts of the response, leading to an orthotropic viscoelastic-viscoplastic model at finite strains. Numerical simulations demonstrate a close match with the experimentally obtained cyclic stress-strain curves across the investigated loading rates.

779	**Sheet Densification and Fiber Bonding as Predictors of Mechanosorptive Creep in Corrugating-Medium Pulps**	Akseli Laatikainen	Contributed talk (12:30-12:45)

T. Harter (1) U. Hirn (1) A. Laatikainen (1)

(1) Institute of Bioproducts and Paper Technology, Graz University of Technology, Inffeldgasse 23, 8010 Graz, Austria

Mechanosorptive creep (MSC), the accelerated time-dependent deformation of paper under simultaneous mechanical load and cyclic humidity, is a leading cause of compressive failure in corrugated containerboard during transport and storage. Despite decades of research, MSC prediction remains challenging because the relative roles of fiber-level hygroexpansion and network-level bonding are still contested. This study systematically compares the cyclic-humidity creep behavior of four industrially relevant corrugating-medium pulps: ammonium-base neutral-sulfite semi-chemical pulp (A-NSSC), sodium-base NSSC (Na-NSSC), eucalyptus high-yield kraft pulp (HY-KP), and recycled old corrugated containerboard (RP). Laboratory handsheets were prepared under two controlled conditions: a fixed-freeness set (Schopper–Riegler 25°) and a fixed-density set (approx. 700 kg/m^3), both achieved through PFI refining. This dual approach decouples fiber-property effects from network-bonding effects on MSC. Compressive creep tests were run under cyclic humidity (50% ↔ 90% RH) until failure, and hygroexpansive strain, sheet density, water retention value, and wet zero-span tensile strength were recorded for each pulp-beating combination. A-NSSC showed the highest MSC resistance across both sets, attributed to its low beating resistance and resulting ability to form

dense, well-bonded fiber networks at moderate refining levels. Time to failure correlated strongly with sheet density (R^2 = 0.87 for virgin pulps), confirming that fiber-fiber bonding governs creep resistance. Hygroexpansive strain, by contrast, showed no positive correlation with MSC. Pulps with the greatest hygroexpansion (A-NSSC) in fact exhibited the longest creep lifetimes. This contradicts earlier reports of a direct positive link between hygroexpansion and MSC acceleration, and is explained by the well-known co-dependence of hygroexpansion on sheet density: denser sheets expand more yet resist creep more effectively through superior bonding. These results establish that network bonding quality is the dominant factor controlling MSC in corrugating-medium pulps, while hygroexpansion alone is not a reliable predictor. Practical improvements to creep resistance should therefore prioritize fiber-fiber bonding and sheet densification over minimizing hygroexpansion.

M37 - Emergent Behavior in Soft and Living Matter

M37 – Session 1 (Fri 25, 10:30-12:30, Chair: Sebastian Fürthauer) Active Matter: Filaments Motility & Living Systems			
ID	Title	Speaker	Type
80	**Embryonic Origami: The forces driving human gastrulation**	Diana Pinheiro	Invited talk (10:30-11:00)

Diana Pinheiro (1)

(1) Research Institute of Molecular Pathology (IMP), Vienna

Gastrulation represents a critical symmetry-breaking event in embryo development, culminating in the specification of all major cell types and the establishment of the body axes. Taking advantage of a two-dimensional (2D) in vitro system derived from human pluripotent stem cells, termed gastruloid discs, we are investigating the molecular and biophysical mechanisms driving human gastrulation. By establishing a high-throughput morphometric pipeline, we found that extraembryonic amnion cells adopt a squamous organization, while the differentiated epiblast remains largely columnar – recapitulating the shape signatures of the 3D human embryo. Through direct force measurements, biophysical modelling, and targeted perturbations, we found that the squamous transition in the amnion is driven by active wetting, i.e. a transition from tension to adhesion dominated cellular states. This is molecularly achieved via the rewiring of cytoskeletal composition in the amnion, from actomyosin to keratin-based networks. We are now investigating whether these shape changes are required for amnion specification and whether they are mechanically transmitted to the embryonic compartment. Overall, this multiscale approach is providing an entry point to understand the regulation and functional role of mechanical forces in human gastrulation.

133	**Phase Separating Nucleator in a Self Straining Active Filament Network**	Jakob Schindelwig	Contributed talk (11:00-11:15)

Quentin Bodini-Lefranc (1,2) Sebastian Fürthauer (1) Jakob Schindelwig (1)

(1) TU Wien
(2) Ecole polytechnique

Many membraneless compartments of cells, such as stress-granules, form via liquid-liquid phase separation. In cells many compartments of the same type and similar sizes can coexist. Since this is inconsistent with equilibrium phase separation physics, we ask if active mechanics could explain this observation. We develop a model coupling dynamics of the droplet material to an active self-straining filament network. This model shows (i) arrested coarsening , (ii) oscillations, (iii) scale selection. We establish that our model is physiologically plausible by comparing to recent work on a phase separating nucleator of actin.

201	**Entropic, Active, and Frictional Forces in Cytoskeletal Crosslinking**	Cedrik Barutel	Contributed talk (11:15-11:30)

Sebastian Fürthauer (1) Cedrik Barutel (1)

(1) TU Wien

The forces that mixtures of motorized and passive crosslinking proteins collectively generate between cytoskeletal filaments within our cells are the key drivers of active cellular mechanics. Despite their importance, a unified theory to describe such crosslinking forces has so far been missing.
I'll show the basis of a theory that predicts the forces generated collectively by crosslinking proteins linking two biopolymer filaments from measurable filament and crosslinker properties, using out-of-equilibrium thermodynamics.
This framework allows us to decompose the forces generated by crosslinkers into three separate components: entropic, active, and frictional. In doing so, it offers a clear physical interpretation of the fundamental mechanisms by which crosslinking proteins self-organize and collectively generate forces.
I'll demonstrate the robustness and utility of this framework by applying it to different experimental observations implying passive and motorized crosslinkers, and disentangle the relative contributions of entropic, active, and frictional forces, clarifying how different physical processes underpin collective force production.

641	**Building a treadmilling filament from the bottom up**	Marija Krstic	Contributed talk (11:30-11:45)

Marija Krstic (1) Christian Vanhille-Campos (2) Buzz Baum (3) Maitane Muñoz-Basagoiti (1) Andela Saric (1)

(1) Institute of Science and Technology Austria
(2) Sorbonne University
(3) MRC Laboratory of Molecular Biology

Many cytoskeletal filaments that drive cellular shape changes and motility, such as actin, FtsZ, and TubZ, undergo treadmilling—a dynamic process in which monomers continuously add to one filament end while dissociating from the other. However, the physical principles that enable treadmilling remain unclear. Treadmilling requires monomer structure to encode faster binding at one filament end to establish directionality. Hydrolysis, modeled as stochastic bond weakening, promotes depolymerization at the opposite end. Because hydrolysis generates a gradient of weakened monomers, filaments must remain stable in the bulk while disassembling at the ends to avoid fragmentation. How single-stranded filaments (e.g., FtsZ) satisfy these competing constraints is unknown.
To probe the single-filament requirements for treadmilling, we construct a colloidal monomer that polymerises into single-stranded filaments and systematically identify the design features required for sustained treadmilling.
We first investigate how directionality can be encoded at the monomer level by analysing binding to a non-hydrolysing filament whose ends are exposed to monomer pools at constant concentration. We find that a way to encode binding kinetics asymmetry is through geometrically modifying the accessible binding area via polymerization, leading to asymmetric growth rates.

We then incorporate hydrolysis by stochastically weakening binding interfaces within the filament. As monomer–monomer binding strength decreases, analysis of filament stability again shows that a two-state system is necessary to stabilise monomers in the filament interior while permitting end disassembly.
Combining these ingredients yields a monomer architecture that exhibits sustained treadmilling dynamics. These results establish general design principles for engineering treadmilling polymers from simple components.

124	**Traveling Wave Dynamics of Microtubule Bed in Drosophila Oocytes**	Alexandra (Olenka) Jain	Contributed talk (11:45-12:00)

Alexandra (Olenka) Jain (1,2) Michael Shelley (2,3) Stanislav Shvartsman (1,2) David Stein (2)

(1) Princeton University
(2) Flatiron Institute, Simons Foundation
(3) Courant Institute, New York University

Cytoplasmic streaming plays a particularly important role in large cells, where the timescales of diffusion are too slow for the mixing and transport of cellular material. The motion of molecular motors on cytoskeletal elements has been known to drive streaming in a variety of biological systems. Previous theoretical studies established that in the Drosophila oocyte, cytoplasmic streaming arises as an instability where normally anchored cortical microtubules (MTs) under compressive loads of molecular motors collectively deform and generate fluid flows. During streaming, the MTs form a globally aligned pattern with two nematic defects. In this paper, we focus on understanding the dynamics of the MT bed that gives rise to streaming in Drosophila oocytes. Using live-imaging and dimensionality reduction techniques, we find a waving regime of MT movement that has yet to be described and quantitatively characterized. We propose an explanation of these waving dynamics in light of our current biophysical model of streaming and we use numerical simulations to find waving behavior at the boundary of two previously characterized regimes. We conclude using both experiments and simulations to suggest that this oscillatory modulation has a function in the mixing of yolk granules, the major source of protein in the early embryo.

629	**Mortal vs immortal filaments: propelled vs growing active matter**	Juraj Majek	Contributed talk (12:00-12:15)

Juraj Májek (1) Edouard Hannezo (1) Andela Šarić (1)

(1) Institute of Science and Technology Austria (ISTA)

Cytoskeletal filaments are vital for various cellular processes, such as cell motility, division and shape maintenance, all of which depend on the active motion of filaments. Across evolution, two mechanisms have emerged: propulsion, in which molecular motors generate an active force; and treadmilling. In treadmilling, filaments directionally polymerize by growing on one end and shrinking on the other, resulting in active motion without any active force. The implications of this mechanism on filament behavior are largely unexplored. Here, we use minimal model simulations to systematically compare treadmilling and propelled filaments, examining their collective behavior, robustness to noise, and interaction with passive objects.
We find that treadmilling and propulsion result in different collision mechanisms: propelled filaments align by mutual pushing, whereas treadmilling depolymerize and “die” upon collision. Both of these collision types can drive collective alignment into filament bundles with nematic (treadmilling) or polar (propelled) symmetry. Treadmilling filaments suppress density fluctuations and therefore require higher density to align, but once aligned, they are far more stable. When a bundle of propelled filaments is locally perturbed, misaligned filaments push against the remaining bundle, causing it to break apart. Perturbed treadmilling filaments simply die out, the perturbation stays local and heals. This results in treadmilling alignment being significantly more robust in crowded and noisy environments. We further ask if these collective states are capable of producing work, placing a passive cogwheel in a bath of filaments. Interestingly, both classes of filaments are capable of rotating the cogwheel, even though treadmilling filaments do not possess any active force. Our findings highlight treadmilling as an alternative mechanism of active motion with robust alignment, revealing design principles of the cytoskeleton and paving the way for novel bioinspired devices.

588	**Training of an Intelligent Triangular Microswimmer Using Genetic Algorithms**	Ruma Maity	Contributed talk (12:15-12:30)

Ruma Maity (1) Maximilian Huebl (2) Julian Lemmel (1) Benedikt Hartl (1) Gerhard Kahl (1)

(1) Technischen Universität Wien
(2) Institute of Science and Technology Austria

Natural microswimmers move in low Reynolds number environments by performing non-reciprocal body deformations that generate propulsion in viscous fluids. Inspired by these mechanisms, artificial microswimmers are being designed to perform tasks such as targeted transport and drug delivery.
In this work, we train a two-dimensional triangular swimmer to move in a desired direction using different propulsion gaits. The swimmer’s dynamics are controlled by adaptive neural networks that map its internal degrees of freedom to applied forces. These networks are optimized using the NEAT (NeuroEvolution of Augmenting Topologies) algorithm, which evolves both the weights and the architecture of the network.
Extending earlier studies [1] on one-dimensional three-bead swimmers navigating chemical landscapes, we consider the more complex case of a two-dimensional triangular swimmer [2]. The system exhibits several emergent non-reciprocal propulsion modes, including flapping, chiral, and walking motions. In two dimensions, a simple reward function based solely on displacement is insufficient to induce effective motion; without a suitable reward scheme, the swimmer tends to remain stationary or move in circular trajectories without net translation. Therefore, a more sophisticated reward function is introduced [2], incorporating instantaneous and average displacement, angular displacement, and shape factors. Analysis of the resulting neural architectures reveals that the emergent networks are relatively simple yet exhibit distinct structural differences corresponding to the various swimming gaits.

1. B. Hartl, M. Hübl, G. Kahl, and A. Zöttl, Proc. Natl. Acad. Sci. USA., 118 (2021), e2019683118.
2. R. Maity, M. Hübl, J. Lemmel, B. Hartl, and G. Kahl, Emergent swimming strategies of an intelligent triangular three-bead swimmer, Submitted.

M37 – Session 2 (Wed 23, 10:30-12:30, Chair: Christos Likos) Active Systems Polymers & Statistical Physics			
ID	Title	Speaker	Type
135	**Tension-based models of epithelial tissues**	Primoz Ziherl	Invited talk (10:30-11:00)

Primoz Ziherl (1,2)

(1) Faculty of Mathematics and Physics, University of Ljubljana
(2) Jozef Stefan Institute

Many mechanical models of tissues are based on the assumption that cells possess an effective surface energy, typically coupled with a hard or a soft volume constraint. In the simplest case, a cell's surface energy differs from that of a liquid droplet only in the magnitude of tensions assigned to its functionally distinct sides. We present a few examples showing how the resulting preferred shape of individual cells, together with an appropriate global constraint such as the volume of the enclosed lumen, gives rise to nontrivial morphologies of single-cell-thick epithelial tissues. We also discuss the relevance of reduced-dimensionality models for describing such tissues.

666	**Adapt & Evolve: How local adaptivity governs global cell behaviour**	Michael Wassermair	Contributed talk (11:00-11:15)

Michael Wassermair (1)

(1) Institute of Science and Technology Austria

Active shape changes are essential for cell function, enabling motility, differentiation, and division. The active processes governing cell shape are tightly regulated by plasma membrane–bound proteins, which enable mechano- and chemosensitive responses as well as adhesion and force transmission to the environment.
We develop a trainable coarse-grained model of a cell that continuously adapts its shape by adapting mechanical properties and activity. Local adaptivity is controlled by artificial neural network policies that capture the dual role of the membrane as both a sensory interface and a coordinator of cell shape.
Using a neuroevolution algorithm, the model learns local adaptation rules that optimize the performance in complex tasks through emergent cooperative behavior of the cells constituent parts. This framework enables agent-based modeling of entire cells and tissues based on decentralized decision-making at the membrane level.
We apply this approach to problems in cell morphology, motility, and tissue formation, demonstrating its ability to inverse-design mechanical parameters for target shapes and to investigate how complex, hierarchical behaviors arise from local interactions and distributed information processing.

195	**How inhomogeneous activity affects the behaviour of active polymers**	Emanuele Locatelli	Contributed talk (11:15-11:30)

Emanuele Locatelli (1)

(1) University of Padova

Active systems, due to the local breaking of equilibrium, allow for phenomena that their equilibrium counterparts cannot attain. For example, polar active polymers, i.e. polymers made of active monomers whose activity is directed as the local tangent to the polymer backbone, display a coil-to-globule-like transition in three dimension, driven by activity. Introducing heterogeneity in the active forces along the backbone considerably affects the polymer substrate. We will discuss three cases: (i) an active-passive diblock, where the position of the block has a strong influence on the polymer, possibly enhancing knot formation[1,2]; (ii) a sinusoidal pattern, where an analytical theory can be worked out for Gaussian polymers[3]; (iii) a dynamic pattern, where active sites are allowed to travel along the chain, mimicking the action of molecular motors[4,5]. We will showcase how each active pattern modifies the conformation and dynamics of the polymers.

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[2] Vatin, M., Orlandini, E., & Locatelli, E. (2025). Upsurge of spontaneous knotting in polar diblock active polymers. Physical Review Letters, 134(16), 168301.
[3] Malgaretti, P., & Locatelli, E. (2025). How Spatially Modulated Activity Reshapes Active Polymer Conformations. arXiv preprint arXiv:2512.14478.
[4] Foglino, M., Locatelli, E., Brackley, C. A., Michieletto, D., Likos, C. N., & Marenduzzo, D. (2019). Non-equilibrium effects of molecular motors on polymers. Soft matter, 15(29), 5995-6005.
[5] Vatin, M. Breoni, et al., Active polymers with migrating active sites, in preparation

478	**Interplay of activity and topology in active polymers**	Davide Breoni	Contributed talk (11:30-11:45)

Davide Breoni (1)

(1) Università di Trento

Polymers present a wide variety of topologies: they can be cyclized, tied into knots, and can form entangled melts. Investigating such structures in the frame of biological systems, we incur into another layer of complexity, as polymers can display activity in the form of directed motion. Studying the interplay of activity and topology in polymers can bring a better understanding of biological system as well as help conceptualize tunable materials. We employ coarse-grained molecular dynamics simulations to study how complex topologies affect systems of tangentially active polymers, focusing on the rheological properties of highly entangled melts and the collapse behavior of knotted rings. We observe that the viscoelastic response of active melts depends marginally on their topology, contrary to passive melts, as energy intake becomes the main driver of the dynamics. Moreover, we find that the melt's rheology can be directly tuned with activity. The opposite behavior is observed in knots, where the role of topology is enhanced by activity: in fact, the collapse transition of active loops depends both on their knot complexity and family, although family has no role in determining the physical properties of passive polymer knots. This study shows that activity and topology heavily affect each other, and that both can be used to tune the properties of complex materials.

271	**Gradient-based optimization of kinetics to enable the design of active multistable systems**	Maximilian Lechner	Contributed talk (11:45-12:00)

Carl Goodrich (1) Maximilian Lechner (1)

(1) Institute of Science and Technology Austria (ISTA)

Biological molecular machines reliably undergo complex nanoscale dynamics to perform tasks, demonstrating how activity and multistability can be harnessed to process information and do work. While it is now possible to engineer complex nanostructures from synthetic building blocks, endowing them with machine-like functionality remains elusive, in part because we lack tools to control their kinetics and tune how they switch between stable states. To take full advantage of our engineering capabilities we need tools that connect the particle level design attributes to the emergent dynamic behavior of assembled systems.
I will show how combining path reweighting, a tool for extrapolating existing simulation data to a modified Hamiltonian, with automatic differentiation makes it possible to compute gradients of dynamical observables, such as transition rates between metastable states, without storing or differentiating through simulation trajectories. This enables the desired functionality of a system to be formulated as an optimization problem and solved using gradient-based methods, providing a principled route to designing systems that switch between target states with prescribed probabilities.
As a proof of concept, I will demonstrate this framework on passive as well as active particles navigating a rugged two-dimensional energy landscape with multiple metastable states. By optimizing the landscape, we can direct the system toward one or several target states with prescribed probabilities, illustrating how rational design principles can be used to encode life-like, adaptive behavior into multistable systems.

483	**Universal Features of a Microscopic Information Engine in Equilibrium**	Remi Goerlich	Contributed talk (12:00-12:15)

Rémi Goerlich (1) Eli Flaxer (1) Gilad Pollack (1) Saar Rahav (1) Yael Roichman (1)

(1) Laboratoire de Physique à l'ENS de Lyon

The ability to measure the stochastic degrees of freedom of a thermal system enables the extraction of energy from an equilibrium heat bath. This is the underlying principle of Maxwell's demon and subsequent information engines [1, 2]. This apparent thermodynamics paradox is resolved when accounting for the energetic cost of the associated information processing and these novel engines are consistently described by the framework of information thermodynamics. Within this frame, it offer new possibilities to control fluctuations as well as energy and information flows through sub-parts of a system. For example, some biological processes at the microscopic scale, such as kinesin cargo-transport use information engine-like mechanism to improve their efficiency [3].
In this work, we experimentally realize a microscopic information engine configured as a compressible piston containing a thermalized colloidal suspension [4]. The particle positions are recorded to identify when a predefined region near the wall is empty, allowing the piston to compress the colloidal suspension without applying work on the system. We find that the mean compression energy W stored is universally set by the probability of a positive measurement outcome by $W = -k_{\mathrm{B}}Tp_1\ln(p_1)$ where p_1 in turn is controlled by parameters such as density and compression step size. We further demonstrate that mechanical work can be extracted during the decompression of the piston, thereby closing the engine's operating cycle. This brings information engine closer to biological system, with a full work-producing cycle at the level of thermal fluctuations.

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528	**The electrostatic nature of protein pair potentials**	Anze Bozic	Contributed talk (12:15-12:30)

Anze Bozic (1)

(1) Jozef Stefan Institue

The electrostatic nature of protein pair potentials dictates the fundamental behavior of biological systems, from molecular recognition to the phase stability of highly concentrated formulations. However, accurately quantifying the effective charge state that governs these potentials remains a challenge, as existing methods often fail to reconcile theoretical predictions with experimental reality. I will present a synergistic framework that resolves the underlying forces of protein association by integrating cryogenic electron tomography with amino-acid-level coarse-grained simulations. By isolating the potentials of mean force (PMF) at specific salt concentrations, this combined approach captures pairwise interactions with exceptional accuracy, enabling a determination of the protein charge state that exceeds the precision of current methods.
The results, validated across hen egg-white and human lysozyme as well as bovine serum albumin, show that the alignment between theory and experiment is uniquely sensitive to the protein's electrostatic environment, while remaining mostly independent of structural variations or non-ionic modifications. Furthermore, the choice of buffer is shown not to be a passive variable but an active modulator of the protein's effective charge, directly shifting the interaction landscape. This methodology allows for a clear mapping of the transition between long-range electrostatic dominance and the emergence of short-range steric and non-ionic forces. By maintaining proteins in their native solution phase, it provides a robust physical foundation for characterization and predictive modeling of protein behavior in complex chemical environments.

M37 – Session 3 (Thu 24, 10:30-12:30, Chair: Emanuela Bianchi) Soft Matter: Self-Assembly Patchy Interactions & Coarse-Grained Modeling			
ID	Title	Speaker	Type
279	**The role of patchy interactions in protein self-assembly and the structural and dynamic properties of high concentration protein solutions**	Peter Schurtenberger	Invited talk (10:30-11:00)

Peter Schurtenberger (1) Fabrizio Camerin (1) Marco Polimeni (2) Emanuela Zaccarelli (3) Anna Stradner (1)

(1) Lund University
(2) University of Copenhagen
(3) Sapienza University of Rome

Protein-protein interactions are known to be often highly anisotropic due to the non-spherical protein shape and inhomogeneities in the distribution of charges and hydrophobic areas on the protein surface. The key static and dynamic properties of concentrated protein solutions and mixtures as those existing in the interior of living cells or used in pharmaceutical formulations are thus strongly dependent on solution parameters such as ionic strength, temperature and pH. Moreover, small variations in the protein structure caused for example by a single point mutation can change their solution behavior dramatically. Key examples are monoclonal antibodies (mAbs), i.e. Y-shaped proteins that have moved into the focus of pharmaceutical industry. While mAbs are central to modern therapeutics, their use is limited by formulation challenges such as high viscosity, aggregation, gelation, opalescence, and phase separation.
Electrostatic interactions fundamentally govern the structure, stability, and dynamics of antibody solutions, yet the impact of heterogeneous and anisotropic charge distributions on their behavior remains elusive. Here, we present results from a combination of scattering experiments, (micro)rheological measurements and simulations. We use a multiscale coarse-graining strategy to interpret data from different mAbs, which allows us to directly connect molecular-level electrostatics to collective solution properties. Our approach provides a predictive pathway to decode and control charge-driven interactions in complex biomolecules and, more generally, in heterogeneously-charged soft matter systems, with immediate relevance to protein formulation and biomaterials engineering.

198	**Extremely coarse-grained modeling of multimeric G-quadruplexes**	Cristiano De Michele	Contributed talk (11:00-11:15)

Cristiano De Michele (1)

(1) "Sapienza" Università di Roma

Biological macromolecules, such as DNA duplexes, proteins and polypeptides, comprise many degree of freedom and live in a water environment. Numerical methods have been widely used to study these biological systems, but many of these methods, such as atomistic molecular dynamics, are rather demanding if many or very large biomolecules are considered. To overcome these limitations, extremely coarse-grained models can be employed, where within these approaches biomolecules retain few degrees of freedom and water is treated implicitly, thus making simulations feasible. A prominent example is provided by G-quadruplexes (G4s), which are helical four-stranded structures forming from guanine-rich nucleic acid sequences and which are thought to play a role in cancer development and malignant transformation. In this seminar I will show examples of extremely coarse-grained modeling of some biomolecules
with special focus on telomeric G4 multimers. Concerning G4s, I will present a novel low-resolution structural approach that combines small-angle X-ray scattering (SAXS) with extremely coarse-grained (ECG) simulations and that allows us to quantify physical properties
of these systems. Complexation of G4 with benchmark ligands, i.e. possible anti-cancer drugs, has been also studied through this approach, proving that it can be an aKordable tool aiding in the selection and design of drugs that target G4s under physiological conditions.

712	**Intercalation and stacking of ligands into patchy polymers**	Flavio Scipione	Contributed talk (11:15-11:30)

Flavio Scipione (1) Cristiano De Michele (2) Emanuela Bianchi (1) Deniz Mostarac (3)

(1) TU Wien
(2) Sapienza, Unviersity of Rome
(3) University of Edingburgh

We introduce a patchy polymer model as a minimal coarse-grained representation of G4 multimers. G4 multimers are chains of G-quadruplexes, which are stable stacks of guanine-rich tetrads. Because they regulate key genomic processes, G4 multimers are promising targets for designing selective therapeutic ligands. A key open question is how ligand binding modifies the mechanical properties of G4 multimers.
While multiscale and fine-grained computational models can accurately capture these systems, they are often too computationally demanding for broad parameter exploration. To overcome this limitation, we use an extremely coarse-grained model and simulate it with a simple Monte Carlo algorithm. Our approach builds on a Kremer–Grest polymer model calibrated to reproduce the known structural and mechanical properties of G4 multimers from fine-grained references. To investigate selective ligand binding, we extend this framework by introducing discrete attractive patches along the polymer backbone. Ligands can bind specifically to these patches rather than interacting uniformly along the chain, allowing us to model intercalation and stacking in a controlled way. Using this toy model, we systematically study how ligand polymerization and interaction parameters control intercalation, stacking and their effects on polymer mechanics. This provides a simple and versatile platform to explore how ligand architecture and binding specificity can be tuned to modulate the structural and mechanical response of G4-based systems.

320	**Steering tetrahedral patchy particles into cubic diamond via external fields**	Lukasz Baran	Contributed talk (11:30-11:45)

Łukasz Baran (1) Edyta Raczyllo (1) Wojciech Rżysko (1) Dariusz Tarasewicz (1)

(1) Maria Curie-Sklodowska University in Lublin

Selective formation of a cubic diamond is challenging due to the formation of competing phases possessing similar free energy. Examples of such are: stacking hybrids of interwoven hexagonal and cubic diamonds with (i) its liquid phase, (ii) arrested glasses, or (iii) clathrates, all depending on the relative patch size, despite being within the single association regime [1, 2]. The necessity to selectively achieve cubic diamond is of paramount importance since it exhibits a complete photonic bandgap at lower frequencies than the hexagonal counterpart, making it a promising candidate in view of photonic applications [3].
Herein, we demonstrate that due to the presence of an external field and by manipulation of its strength we can attain selectivity in the formation of a cubic diamond in a one-component system comprised of designer tetrahedral patchy particles, despite the formation of stacking hybrids in bulk. The driving force of such a phenomenon is the structure of the first adlayer which is commensurate with the (110) face of the cubic diamond [4].
In contrast, we show that the 1:1 mixture of identical patchy particles cannot selectively form the cubic diamond and always yields a mixture of both diamond phases, however, the emergence of stacking hybrids is observed for a wider range of patch sizes compared to the one-component system [5]. The reason for such a change in the growth mechanism is due to the frustrations present in the system that are manifested in the primary adsorption layer and propagate as the film grows.

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[5] D.Tarasewicz, E. Raczyłło, W. Rżysko, Ł. Baran, Self-assembly of chromatic patchy particles with tetrahedrally arranged patches, Soft Matter 21, 1203-1211 (2025).

745	**Effective interaction between two charged Janus colloids in an asymmetric ionic solution**	Natasa Adzic	Contributed talk (11:45-12:00)

Natasa Adzic (1) Emanuela Bianchi (2)

(1) Institute of Physics Belgrade, University of Belgrade, Serbia
(2) TU Wien

Recent studies of electrostatics in colloidal systems have increasingly addressed the complexity that inhomogeneous surface charge distributions introduce into self-assembly processes. However, approaches based on extensions of DLVO-like models remain valid only within the mean-field regime and are therefore mainly applicable to environments dominated by monovalent salts, [1]. In the work we present, we move beyond this limitation by developing a theory for anisotropically charged colloids that is applicable in regimes where mean-field theory fails, such as in salt mixtures containing polyvalent ions. When polyvalent ions are present, strong coupling effects emerge, leading to unconventional electrostatic phenomena such as like-charge attraction. While these effects are well documented for uniformly charged systems, their role in systems with anisotropic charge distributions remains largely unexplored.
To address this problem, we consider a simplified model of Janus colloids immersed in a mixed ionic solution containing both monovalent and multivalent salts. Using a field-theoretic, path-integral approach, we derive effective electrostatic interactions that explicitly account for strong correlations and ionic asymmetry. This framework enables exploration of the full orientational dependence of pair interactions and provides a foundation for incorporating these effects into coarse-grained simulations. Our results contribute to a more comprehensive understanding of electrostatic self-assembly in complex ionic environments.

[1] A. Gnidovec, E. Localtelli, S. Čopar, A. Božič and E. Bianchi, Natt. Comm., 16, 4277, 2025.

756	**Geometric principles for the design of self-assembling flexible subunits**	Botond Tyukodi	Contributed talk (12:00-12:15)

Botond Tyukodi (1) Fernando Caballero (2) Gregory Grason (3) Michael Hagan (2) Douglas Hall (3) Daichi Hayakawa (2) W. Benjamin Rogers (2)

(1) Babes Bolyai University
(2) Brandeis University
(3) UMass Amherst

Recent advances in synthetic methods enable designing subunits that self-assemble into structures with precise, finite sizes and well-defined architectures, but yields are frequently suppressed by the formation of off-target metastable structures. Increasing the complexity (the number of distinct subunit types) can inhibit off-target structures, but leads to slower kinetics and higher synthesis costs. Here, we study icosahedral shells formed of programmable triangular subunits as a model system, and identify design principles that produce the highest target yield at the lowest complexity.
We use a symmetry-based construction to create a range of design complexities, starting from the maximal symmetry Caspar-Klug assembly up to the fully addressable, zero-symmetry assembly. Kinetic Monte Carlo simulations reveal that the most prominent defects leading to off-target assemblies are disclinations at sites of rotational symmetry. We derive symmetry-based rules for identifying the optimal (lowest-complexity, highest-symmetry) design that inhibits these disclinations, leading to robust, high-fidelity assembly of targets with arbitrarily large, yet precise, finite sizes. The optimal complexity varies non-monotonically with target size, with `magic' sizes appearing for high-symmetry designs in which symmetry axes do not intersect vertices of the triangular net. The optimal designs at magic sizes require 12 times fewer inequivalent interaction-types than the (minimal symmetry) fully addressable construction, which greatly reduces the timescale and experimental cost required to achieve high fidelity assembly of large targets. This symmetry-based principle for pruning off-target assembly generalizes to diverse architectures with different topologies.

M37 – Poster session (PS2 Wed23-Fri25)			
ID	Title	Presenter	Type
70 **P075**	**Emergent Interactions in Active Droplets- Non Reciprocal Interaction In Liquid Crystal Droplets**	Nihal Ibrahim P P	Poster

Nihal Ibrahim P P (1)

(1) National Centre for Biological Sciences (NCBS), Bangalore

Active matter consists of many individual units that continuously consume energy to move or generate mechanical forces. These systems exhibit rich collective behaviors arising from interactions between their components. A particularly interesting class of interactions in active matter is non-reciprocal interactions, where the force exerted by particle i on particle j is not equal and opposite to the force exerted by j on i. This effectively breaks Newton's third law at the coarse-grained level and gives rise to behaviors that are not possible in equilibrium systems. A well-known example of such non-reciprocal interaction is the predator–prey interaction, where the predator is attracted to the prey while the prey is repelled by the predator.
In this thesis, we investigate emergent interactions in active liquid crystal droplets. The experiments are conducted in a quasi-two-dimensional flow cell constructed using double-sided adhesive tape with a thickness of 50 µm. These liquid crystals are known to exhibit thermally reversible phase transitions from smectic to nematic to isotropic phases. Monodisperse droplets are generated using flow-focusing microfluidic devices, and epifluorescence microscopy is employed to track internal flows, interfacial behavior, and droplet shape dynamics.
We observe a predator–prey-like mechanism in liquid crystal droplets dispersed in Triton X surfactant solutions. Specifically, we work with 5CB (4-cyano-4'-pentylbiphenyl) and 8CB (4-cyano-4'-octylbiphenyl) droplets of approximately 50 µm diameter in non-ionic surfactant solutions. We first characterized the solubilization rates of individual droplets in both non-ionic and ionic surfactants. To identify material transfer between 5CB and 8CB droplets, one population of droplets was labeled with Nile Red dye. Over time, fluorescence was observed in initially unlabeled droplets, confirming inter-droplet material transfer. We then studied the solubilization dynamics in mixed droplet environments and compared them with the behavior of isolated droplets.
Our results show that 8CB droplets grow over time, while 5CB droplets shrink, establishing a predator–prey analogy in which 8CB acts as the predator and 5CB as the prey. We further investigate the effect of surfactant concentration on material transfer and interaction dynamics. Using a temperature-controlled stage (CherryTemp), we study the influence of temperature on the rate of interaction. Additionally, we analyze how the coordination number affects droplet assembly and the velocity of collective organization.
Future work will focus on further characterization of this system in Triton X surfactant, followed by extension to other surfactant systems. We aim to investigate whether the observed behavior is reversible and to understand the differences arising from the use of different surfactants, as well as to explore potential applications of these non-reciprocal active droplet systems

71 **P076**	**From LRO to Disorder via QLRO in Spatially Inhomogeneous Polar Flock**	Anish Kumar	Poster

Anish Kumar (1) Vivek Semwal (2) Shradha Mishra (1)

(1) Indian Institute of Technology (BHU) Varanasi
(2) RIKEN Center for Biosystems Dynamics Research, Kobe, Japan

We study the collective behavior of a polar flock in an inhomogeneous environment in two dimensions. The inhomogeneity is modeled by introducing circular regions at random locations on the substrate with high noise, but accessible for the flock to move. Hence, inside such regions, the particles' orientation gets randomized. Such inhomogeneities differ from physical disorder, which obstructs the space for incoming particles. The study focuses on how the phase behavior of polar flock changes by tuning the area fraction of inhomogeneity. As area fraction increases, the system crosses over from long-range to quasi-long-range order and ultimately to a disordered phase, while the order–disorder transition for flocking changes from discontinuous to continuous.

406 **P077**	**Active Taylor Dispersion of E. coli: Effects of Chirality and Time-Periodic Flow in Microchannels**	Stephan Hufnagl	Poster

Stephan Hufnagl (1,2) Andreas Zöttl (1)

(1) Faculty of Physics, University of Vienna
(2) Vienna Doctoral School in Physics

Active matter, consisting of self-propelled particles and swimming microorganisms, demonstrates complex dynamics in flow environments. These dynamics are essential for understanding both biological and technical systems. We present computational results on the dynamics and active Taylor dispersion of swimming E. coli bacteria in 3D microchannel Poiseuille flow under varying Péclet numbers, which correspond to different flow conditions and lead to distinct diffusive regimes.
We first recover by applying a steady Poiseuille flow classical Taylor dispersion of passive particles, as well as active Taylor dispersion of active Brownian particles. We then demonstrate the effect of bacterial chirality on the effective diffusion, which reduces long-time diffusion but shows similar scaling with increase of Péclet as for non-chiral microswimmers. We further discuss the influence of time-periodic flow on the dispersion of swimming bacteria, introducing an additional time scale to the system.

741 **P078**	**Distinct filament kinetics, unified defect dynamics in active nematics**	Kseniia Petukhova	Poster

Andraz Gnidovec (1) Juraj Májek (1) Kseniia Petukhova (1) Andela Šarić (1)

(1) Institute of Science and Technology Austria (ISTA)

Topological defects govern the large-scale dynamics of active nematic systems, yet their behavior depends sensitively on the underlying filament kinetics. In particular, treadmilling and stochastic growth–shrinkage (catastrophe) represent distinct microscopic mechanisms that generate active stresses, raising the question of how these dynamics influence defect evolution and system ordering.

Here, we compare active nematic systems composed of treadmilling filaments and filaments undergoing catastrophic dynamics using numerical simulations. We quantify defect coarsening, global nematic order, and filament statistics across a range of conditions.
We observe that defect density decays in time following a scaling law, with comparable coarsening behavior between the two systems within current estimates. Treadmilling systems exhibit higher nematic order and shorter, more uniform filament lengths, while catastrophic dynamics lead to longer filaments and increased disorder. Despite these differences, we identify an effective length scale that collapses the ordering behavior of both systems onto a universal curve.
We further quantify defect–defect interactions through analysis of defect trajectories and pair statistics, linking microscopic filament kinetics to emergent collective dynamics. These results provide a unified framework for understanding how filament turnover mechanisms control topological defect behavior in active materials and biological systems.

M38 - Astronomy and Astrophysics across Austria

M38 – Session 1 (Thu 24, 10:30-12:30)			
ID	Title	Speaker	Type
258	**Astrophysical Research at the Universität Innsbruck highlighting pre-main sequence asteroseismology**	Konstanze Zwintz	Invited talk (10:30-10:55)

Konstanze Zwintz (1)

(1) Universität Innsbruck

At the Institute for Astro- and Particle Physics of the Universität Innsbruck, astrophysical research revolves around galactic and extragalactic topics including different phases of stellar evolution, stellar oscillations, massive stars, galaxy formation and evolution, and cosmology.
In my talk I will first give a short overview about the research groups at my institute. I will then introduce pre-main sequence asteroseismology - the research conducted in my group "Stellar evolution and asteroseismology". I will also show our contributions to the ESA mission PLATO which is expected to be launched in early 2027.

222	**Gravitational-wave and electromagnetic signatures of binary black holes with circumbinary gas**	Zoltan Haiman	Invited talk (10:55-11:20)

Zoltan Haiman (1)

(1) Institute of Science and Technology Austria (ISTA)

Binary black holes (BHBs) embedded in dense gas hold the promise of "multi-messenger astrophysics": when they are detected both through gravitational waves (GWs) and electromagnetic (EM) observations, they will enable novel science. This is true both for massive BHBs, whose GWs will be detectable by the future LISA satellite and by on-going pulsar timing arrays (PTAs), as well as for stellar-mass BHBs detected through ground-based GW detectors. In both cases, identifying coalescing binaries through their EM signatures will help clarify their astrophysical origin and yield novel probes of cosmology, fundamental physics, and accretion physics. In this talk, I will describe how circumbinary gas may impact the orbital evoluton of binaries, while producing characteristic EM signatures for both massive and stellar-mass BHBs, based on hydrodynamical simulations and analytic models. In both cases, several binary candidates have been identified in optical surveys, and LSST should soon be able to uncover robust binaries based on their high-quality, multi-band light-curves.

168	**Connecting solar and in-situ properties of coronal mass ejections**	Manuela Temmer	Contributed talk (11:20-11:32)

Manuela Temmer (1)

(1) University of Graz

Coronal Mass Ejections (CMEs) are massive eruptions of plasma and magnetic fields from the Sun, capable of impacting Earth's space weather environment. Understanding their evolution from the Sun to interplanetary space requires connecting solar-origin observations to in-situ measurements. This talk covers investigations on the relationships between CME properties, such as speed, magnetic field structure, and plasma density, as observed in remote sensing image data and their counterparts detected in-situ by spacecraft. Specifically, we focus on the examination of the role of solar wind and interplanetary magnetic field interactions in shaping CME dynamics. These results also provide new insights in how solar magnetic fields and plasma conditions govern the geoeffectiveness of CMEs.

247	**Magnetic Topology and Loop Statistics in Observed Coronal Holes Using Potential Field Modeling**	Manuela Temmer	Contributed talk (11:32-11:44)

Stephan Heinemann (1) Jens Pomoell (2) Manuela Temmer (1)

(1) University of Graz
(2) University of Helsinki

Despite its role as the primary model for mapping solar wind sources, the Potential Field Source Surface (PFSS) model consistently fails to replicate the observed boundaries and internal topologies of coronal holes (CHs). To address this, we present a comprehensive statistical analysis of 702 observed CHs from 2010–2019, contrasting their PFSS-modeled magnetic structure with those of Quiet Sun (QS) regions.
Our results reveal a distinct low-altitude magnetic signature within CH boundaries: low-lying loops that are statistically narrower and lower than in the QS, with a median height that is strongly correlated to the mean magnetic flux density (cc = 0.81) in CHs, a relationship not present in QS areas. This suggests that CH magnetic topology is highly sensitive to local flux variations, which is often lost in global extrapolations. We also identify a distinct population of loops within CHs that reach high into the corona. This suggests that a single, global source surface radius (R_ss) is fundamentally inadequate for capturing CH connectivity.
Critically, we find that the model retains distinct structural differences between CH and QS regions even when it fails to predict open flux. Our results demonstrate that the mismatch between models and observations stems from inherent modeling limitations rather than observational error. To better capture the observed open field structure while maintaining computational efficiency, future modeling efforts should transition toward spatially-adaptive or non-uniform source surfaces that respond to local magnetic configurations.

217	**Probing the solar corona with the Solar Orbiter/Metis coronagraph: from instrumentation to CME diagnostics**	Yara De Leo	Contributed talk (11:44-11:56)

Yara De Leo (1,2) Manuela Temmer (2)

(1) INAF- Astrophysical Observatory of Catania (Italy)
(2) University of Graz (Austria)

The Solar Orbiter mission has significantly advanced the study of the solar corona and its connection to the heliosphere through its unique orbital configuration and state-of-the-art instrumentation. Among its remote-sensing payload, the SolO/Metis coronagraph provides, for the first time, simultaneous two-dimensional imaging of the extended solar corona in visible light (VL) and ultraviolet (UV) H I Ly-α emission. This dual-channel capability enables novel diagnostics of coronal plasma, bridging observations from the inner to the middle corona and offering new insights into the origin and evolution of coronal mass ejections (CMEs) and eruptive prominences.
The quantitative exploitation of Metis observations relies on a robust radiometric calibration of its dual channels. In-flight calibration strategies based on stellar observations enable the determination of absolute coronal brightness and the monitoring of instrumental stability over time. This calibration framework provides the foundation for reliable plasma diagnostics and ensures consistency with complementary observations from other instruments.
Metis data enable the application of advanced three-dimensional CME reconstruction techniques, including tie-point triangulation, the Graduated Cylindrical Shell model, and the polarization ratio technique. The combination of these methods allows the reconstruction of CME morphology and propagation in three dimensions, as well as the derivation of key plasma parameters such as electron density and mass, which are essential for characterizing CME dynamics and energetics.
A representative example is provided by the analysis of two CMEs observed on 28 October 2021. These events, characterized by exceptionally bright ultraviolet emission from erupting prominences, were investigated through a comprehensive multi-instrument dataset including STEREO-A, SDO, SOHO, PROBA-2, and ground-based H-α observations. The analysis revealed distinct eruption scenarios, ranging from a slow three-part CME associated with a quiescent filament to a fast halo CME originating from an active region. These events provided a testbed for validating the combined use of 3D reconstruction techniques and plasma diagnostics, demonstrating the capability of Metis to track prominence material to large heliocentric distances and to constrain CME physical properties.
A complementary approach exploits the synergy between Metis and the EUI/FSI instrument to achieve seamless tracking of eruptive prominences across the transition from the low to the middle corona. The development of the EUIMET tool enables the construction of continuous mosaics combining extreme-ultraviolet and coronagraphic observations, incorporating advanced image enhancement techniques and configurable opacity levels. This methodology has been applied to the polar crown eruption of 20 April 2023, providing a unified morphological and kinematic characterization of the event through triangulation and time–distance analysis, and demonstrating the potential for systematic multi-wavelength investigations of CME initiation and early propagation.
Overall, the combination of calibrated multi-wavelength observations, advanced three-dimensional reconstruction techniques, and dedicated analysis tools establishes Solar Orbiter Metis as a powerful diagnostic platform for investigating CME evolution. In particular, its unique capability to simultaneously observe the coronal plasma in VL and UV emission, at high spatial and temporal resolutions, provides unprecedented access to the fine structure of CMEs, including the detailed morphology and thermodynamic properties of erupting prominence material and internal substructures. These capabilities contribute to bridging the gap between the low corona and the heliosphere, improving the understanding of the physical processes governing coronal transients, and supporting future developments in heliospheric research and space weather forecasting.

248	**Spectral signatures from faculae in line-by-line RV**	Sowmya Krishnamurthy	Contributed talk (11:56-12:08)

Florian Kröll (1) Sowmya Krishnamurthy (1)

(1) University of Graz

Radial velocity (RV) searches for small exoplanets around Sun-like stars are increasingly limited by activity-driven RV jitter. In stars with near-solar magnetic activity, bright faculae dominate this variability, yet their disk-integrated RV impact is poorly constrained. In this study, we measure their spectroscopic imprint with a physically consistent forward model, using the Sun as a testing bed.
We compute high-resolution synthetic spectra for a grid of viewing angles using the MPS-ATLAS radiative transfer code and 3D radiative MHD MURaM simulations of the quiet Sun and faculae. We then model the transit of a simple facular patch at the solar equator as the Sun rotates and analyse its signatures in a small sample of disk-integrated FeI and FeII line profiles.
Our results reveal that the strongly μ-dependent suppression of convective blueshift by faculae leads to characteristic RV profiles. Near disk centre the signal is dominated by reduced vertical blueshift, yielding a relative redshift, whereas toward the limb horizontal inflows into facular flux tubes and the enhanced weight of the approaching hot wall produce a relative blueshift despite foreshortening. We find that stellar rotation introduces asymmetry and shifts the RV extrema in phase, producing a facular-transit phase lag that is observed on the Sun and varies from line to line. RV amplitudes depend strongly on both line strength and ionisation stage, with the largest signals generally found for FeII lines and for weaker lines in both FeI and FeII.
Even a single facular region can therefore generate complex, position- and line-dependent RV signatures, motivating line-by-line RV extraction and activity-informed line weighting for extreme-precision RV surveys.

376	**Conditioning of the solar corona by large flares**	Julia Thalmann	Contributed talk (12:08-12:20)

Julia Thalmann (1) Manu Gupta (1) Yang Liu (2) Astrid Veronig (1)

(1) University of Graz
(2) Stanford University

We study the conditions of the solar corona with respect to the occurrence of confined and eruptive (CME-associated) large flares. We model the coronal evolution around 231 large flares observed during solar cycle 24. Based on nonlinear force-free magnetic field extrapolations, we approximate the coronal energy and helicity budgets of the flares' source regions. In particular, we study the characteristics of the pre- and post-flare time evolution of magnetic-field related quantities, including the free magnetic energy and magnetic helicity. We find that during the 24 hours leading to a major flare, the total magnetic energy and unsigned magnetic flux evolve closely with respect to each other -- irrespective of the flare type (confined or eruptive). Prior to confined flares, the free magnetic energy evolves in a way that exhibits more of a similarity with the photospheric unsigned flux than the helicity of the current-carrying field,

while the opposite is observed prior to eruptive flares. The coronal energy and helicity budgets return to preflare levels within six to twelve hours or more, serving as a partial explanation for the rare observation of successive eruptive major flares within a time frame of a few hours.

318	**Coronal dimmings and their relevance for solar and stellar coronal mass ejections**	Astrid Veronig	Contributed talk (12:20-12:32)

Astrid Veronig (1)

(1) University of Graz

Coronal dimmings are transient decreases of the coronal brightness observed in extreme ultraviolet (EUV) and soft X-ray (SXR) wavelengths that occur during the initial stages of a coronal mass ejection (CME). Coronal dimmings are an effect of field line opening, expansion and mass loss during a CME. However, their diagnostics potential reaches far beyond those aspects.
In this contribution, we will present selected results along three main lines:
1. how coronal dimmings are related to decisive properties of a CME,
2. how they can give us insight into the magnetic flux systems that are involved in the eruption,
3. and how they can be used to detect and characterize stellar coronal mass ejections.

M38 – Session 2 (Thu 24, 16:00-18:00)

ID	Title	Speaker	Type
235	**Climate regimes on extrasolar planets**	Christiane Helling	Invited talk (16:00-16:25)

Christiane Helling (1)

(1) Space Research Institute, Austrian Academy of Sciences (ÖAW)

The ensemble of the more than 6000 known extrasolar planets in our galaxy exhibits a diversity of objects unseen in our solar system. Exoplanet research has therefore turned from discovering such planets outside the solar system to characterizing these objects that orbit stars other than the Sun. Recent progress in characterizing exoplanets with the CHEOPS, TESS, and JWST space telescopes has demonstrated that extrasolar gas giants exhibit climate regimes ranging from ultra-hot to rather cold. Ultra-hot Jupiters (like WASP-18b and Kelt-7b) exhibit enormous day-nigh temperature different of more than 2000K. Strong eastward wind jets therefore transport hot gases from the dayside to the nightside where mineral cloud particles form.
The resulting chemical asymmetries are observable with space telescopes like JWST but also PLATO in the future and may be used to characterize exoplanet climate regimes. In order to physically interpret such complex atmosphere behavior, our research group has build virtual laboratories that enable us to predict temperature, velocity, cloud and chemistry maps for planets orbiting different host stars. Such virtual laboratories that describe and explore the atmosphere structure and cloud formation allow us detailed studies of specific planets (e.g. the JWST target WASP-39b) as well as ensemble studies, for example, in preparation of observational campaigns. This talk will present some of our most resent works on exoplanet climate characterisation.

391	**Protoplanetary Disks: From Star Formation to Planetary Systems**	Kundan Kadam	Contributed talk (16:25-16:37)

Kundan Kadam (1)

(1) Space Research Institute, Austrian Academy of Sciences (IWF, ÖAW)

Protoplanetary disks are the natural outcome of low-mass star formation and the environments within which planets are born. In the classical picture, a collapsing molecular cloud core gives rise to a protostar surrounded by a centrifugally supported disk, where submicron-sized dust grains grow and eventually assemble into planetary systems. Disk evolution is regulated by angular momentum transport through viscous and gravitational torques, as well as by mass and angular momentum loss in magnetically driven disk winds. In reality, however, these disks are shaped by a rich interplay of physical processes, including dust-gas dynamics, magnetohydrodynamics, volatile transport, external photoevaporation, chemistry, and disk instabilities.
In this talk, I will discuss how these processes influence the formation and long-term evolution of protoplanetary disks, and how they affect the environments in which planets form. I will highlight my work on theoretical and hydrodynamic modeling of disks, with an emphasis on connecting models to observations from current and future ground- and space-based facilities.

390	**Models of heating and diffusive processes in the solar corona**	Philippe Bourdin	Contributed talk (16:37-16:49)

Philippe Bourdin (1)

(1) University of Graz

It is a challenge to construct models of realistic phenomena in the solar corona, but it is a requirement to validate the model results against real observed structures, such as coronal EUV-bright loops and coronal Doppler shifts. On the one hand, if we aim to include self-consistently driven convection below the photosphere to have a realistic driving, the photospheric magnetic field is likely not the same as in the real photosphere. On the other hand, when we prescribe realistic vertical magnetic fields in the photosphere, the convection can not be included and an artificial granulation driver has to be implemented. While the former can never exactly reproduce the photospheric conditions and hence structures in the corona, the latter has at least a chance if the granulation driver is realistic enough. Further complications arise from numerical necessities such as explicit diffusivity in the MHD equations, such as the viscosity, the heat conduction, and the magnetic diffusivity. Those diffusivities are needed to keep numerical errors under a controlled and insignificant level. In this work we discuss how such diffusivities need to be chosen according to the grid spacing. This allows us to simulate a large coronal EUV-bright loop between two pores, where we also see some match to observed Doppler shifts in Fe-XII.

761	**Evolution of Galaxy Scaling Relations**	Bodo Ziegler	Invited talk (17:00-17:25)

Bodo Ziegler (1)

(1) University of Vienna

Galaxies obey scaling relations between global physical properties like stellar mass-size, mass-star formation rate, and mass-gas metallicity. Exploiting kinematics as proxy for total mass relations between the baryonic components and the dark matter can be explored like the Tully-Fisher or Fundamental Plane relations. Such scaling relations allow to measure galaxy evolution across cosmic epochs in a quantitative way. In addition, they serve as benchmarks to verify predictions from simulations.

702	**A high precision mass measurement of the central black hole in the massive elliptical galaxy NGC 2513 with ALMA molecular gas dynamics**	Shelley-Anne Harrisberg	Contributed talk (17:25-17:37)

Shelley-Anne Harrisberg (1) Alvaro Hacar (1) Hai N. Ngo (2) Dieu D. Nguyen (3) Sabine Thater (1)

(1) Department of Astronomy, University of Vienna
(2) Faculty of Physics – Engineering Physics, University of Science, Vietnam National University
(3) Department of Astronomy, University of Michigan

Supermassive black holes (SMBH) are believed to co-evolve with their host galaxies. Evidence for this coevolution is found in the form of several correlations between the SMBH mass and various properties of the host galaxy, the tightest of which is the bulge stellar velocity dispersion (e.g., Ferrarese & Merritt 2000). To better understand these correlations, a large and robust dataset of SMBH measurements is required, particularly in the low- and high-mass regime where measurements are still relatively few. In this talk, I present the results of a mass measurement of the putative SMBH in the massive elliptical galaxy NGC 2513. The measurement was obtained via the method of cold molecular gas dynamics (Davis et al. 2013) using high resolution ALMA (Atacama Large Millimetre/sub-millimetre Array) observations. I briefly introduce the method and then present how I derived the luminous mass using near-infrared images fromm the Hubble Space Telescope, taking dust masking into account and noting that an accurate knowledge of the galaxy's luminous mass is crucial towards obtaining a precise SMBH mass measurement. I subsequently explain how I combined different 12CO(2-1) ALMA observations to obtain the highest possible resolution at a sufficient sensitivity. Finally, I discuss the modelling of the resulting ALMA datacube with the KINematic Molecular Simulation (KinMS) routines developed by Davis et al. (2012) to obtain a best-fit model and SMBH mass. I conclude by examining my results with respect to the correlation mentioned above and discuss outlooks for this project and future study in the field.

667	**Systematic Search for Local Little Red Dots in DESI DR1**	Kevin Park	Contributed talk (17:37-17:49)

Sara Mascia (1) Jorryt Matthee (1) Kevin Park (1) Alberto Torralba (1)

(1) Institute of Science and Technology Austria (ISTA)

JWST has unveiled an abundant population of compact broad-line emitters at $z \gtrsim 4$, the Little Red Dots (LRDs), which might represent a previously unprobed supermassive black hole (SMBH) evolution channel predominant at high redshift. However, the LRDs have remained mostly elusive at lower redshift ($z \lesssim 0.5$) where detailed studies are possible from ground-based observatories.
We searched for local Little Red Dots (LRDs) in the catalog of the Dark Energy Spectroscopic Instrument (DESI) based on emission line properties, as opposed to earlier approaches that searched for specific spectral energy distributions in photometry. We report the discovery of eight local LRDs at $z = 0.2 - 0.45$, which show similar properties to the high-redshift LRDs in the rest-frame optical. The eight sources are characterized by broad Balmer lines and compact morphologies like their high-redshift counterparts, also showing Balmer absorption features and/or strong He I emission, but weak HeII or other high excitation lines. For 7 out of 8 sources, we retrieve light curves from time-domain surveys and find weak to none intrinsic variability ($0.0 - 0.1$ mag) over several years in the rest-frame. During our search, we find an AGN which shows analogous features to our sources and we discuss its properties in comparison to LRDs. Given the effective area covered by DESI DR1 (~ 9500 deg^2), our sample roughly corresponds to a number density of 1.6×10^{-9} Mpc^{-3} at $z < 0.45$, confirming about 10,000 lower number densities than in the first billion years of cosmic time.

44	**Geodesics v.s. q-Desics: On the Motion in Quantum-Gravitational Background**	Benjamin Koch	Contributed talk (17:49-18:01)

Benjamin Koch (1) Ali Riahinia (1)

(1) TU Vienna

We investigate the motion of test particles in quantum-gravitational backgrounds by introducing the concept of q–desics, quantum-corrected analogs of classical geodesics. Unlike standard approaches that rely solely on the expectation value of the spacetime metric, our formulation is based on the expectation value of quantum operators, such as the affine connection operator. This allows us to capture richer geometric information. We derive the q–desic equation using both Lagrangian and Hamiltonian methods and apply it to spherically symmetric static backgrounds obtained from canonical quantum gravity. Exemplary results include lightlike radial motion and circular motion with quantum gravitational corrections far above the Planck scale. This framework provides a refined description of motion in quantum spacetimes and opens new directions for probing the interface between quantum gravity and classical general relativity.

M39 - Next Generation Gravitational Wave Observations

M39 – Session 1 (Mon 21, 10:30-12:30, Chair: Axel Maas)			
ID	Title	Speaker	Type
646	**Einstein Telescope, pushing the outer limits of gravitational waves detection**	Angelique Lartaux	Invited talk (10:30-11:00)

Angelique Lartaux (1)

(1) CNRS/IJCLab

Einstein Telescope is the next generation ground based European gravitational-wave detector that will change the paradigm of gravitational wave detection to routine observations and with observable signals up to the Universe's first moments. To reach this goal, an increase of sensitivity by at least a factor of ten with respect to the current generation gravitational-wave detectors' final design will be needed.
In this presentation I will give an overview of some instrumental challenges to reach such precision in the measurement.

656	**The Einstein Telescope: challenges and opportunities of a third-generation detector**	Filippo Santoliquido	Invited talk (11:00-11:30)

Filippo Santoliquido (1)

(1) Gran Sasso Science Institute (GSSI)

The Einstein Telescope (ET) is a European project for a third-generation gravitational-wave detector designed to increase the sensitivity of present interferometers by approximately one order of magnitude. Two reference designs are currently under investigation: a triangular-shaped detector with 10 km arms, and a configuration with two L-shaped detectors with 15 km arms, both located in Europe. Each arm will host a 'xylophone' setup of two interferometers: one optimized for high frequencies, the other, cryogenic, for low frequencies. This design will significantly expand the observable volume of the Universe and improve source parameter estimation. In this contribution, I will outline the scientific program of the ET, tracing the project's evolution, current status, and prospects. We give an overview of the technological challenges, especially for the low-frequency instrument, and the scientific reach of a third-generation detector like ET, highlighting the potential for discoveries in fundamental physics, multi-messenger astrophysics, and cosmology.

651	**Exploring fundamental physics with Einstein Telescope**	Francesco Crescimbeni	Invited talk (11:30-11:50)

Francesco Crescimbeni (1)

(1) Sapienza University of Rome

Gravitational waves have opened a new observational window onto the astrophysics of compact objects. With next-generation detectors such as the Einstein Telescope, General Relativity (GR) and the nature of compact objects will be probed with unprecedented precision.
In this talk, building on the activities of the Fundamental Physics division of the Einstein Telescope Collaboration, I will present an overview of current and future tests of General Relativity, highlighting potential "smoking gun" signatures of beyond-GR effects in both the inspiral and ringdown phases.

765	**Probing intermediate-mass black hole assembly in star clusters with gravitational waves**	Lavinia Paiella	Invited talk (11:50-12:10)

Lavinia Paiella (1)

(1) Gran Sasso Science Institute (GSSI)

Intermediate-mass black holes (IMBHs), expected to occupy the mass range between stellar-mass and supermassive black holes (approximately 100-10000 solar masses), remain one of the least explored populations of compact objects. Dense star clusters are thought to play a central role in their formation, with stars and stellar-mass black holes acting as the primary building blocks. These environments produce binaries that can eventually be detected through gravitational-wave observations.
In this talk, I will explore the conditions under which IMBHs can form in star clusters through runaway stellar mergers and hierarchical binary black hole mergers. I will present results from a suite of simulations performed with the semi-analytic population synthesis code B-POP, focusing on the efficiency of IMBH formation and the production of intermediate mass-ratio inspirals.
I will also discuss the possible dynamical origin of the recent candidate event GW231123, reported by the LIGO-Virgo-KAGRA (LVK) collaboration, which may represent the first evidence of a light IMBH binary merger.
Finally, I will highlight how these simulations improve our understanding of the dynamical contribution to the observed population of binary black hole mergers and help assess the prospects for detecting IMBHs with future third-generation gravitational-wave observatories such as the Einstein Telescope.

	Discussion		(20 min.)

M39 – Session 2 (Mon 21, 16:00-18:00, Chair: Ulyana Dupletsa)			
ID	Title	Speaker	Type
665	**Gravitational waves as a probe of stellar and galaxy evolution in the next-generation detector era**	Martyna Chruslinska	Invited talk (16:00-16:20)

Martyna Chruslinska (1)

(1) European Southern Observatory (ESO)

Gravitational-wave astronomy is entering a new regime: as current detectors improve and the next generation of ground-based facilities comes online, detection rates of stellar-mass compact-object mergers will increase from hundreds to millions per year. The observed merger population will comprise systems formed across cosmic time, originating from stars born with different chemical compositions and in a wide range of galactic environments.
I will discuss how this represents both an opportunity and a challenge. On the one hand, gravitational-wave observations provide a powerful new probe of how massive stars form and evolve in environments very different from our own Galaxy. They can also offer complementary constraints on cosmic chemical evolution and star formation beyond the reach of electromagnetic observations. On the other hand, interpreting these populations is highly non-trivial, as different merger formation channels and uncertainties in the evolving cosmic environment can produce degenerate observable signatures.
I will reflect on how the information provided by future detectors can help overcome these challenges and unlock the astrophysical information encoded in gravitational-wave populations.

679	**Why are stellar models overestimating binary black hole mergers?**	Cecilia Sgalletta	Contributed talk (16:20-16:40)

Cecilia Sgalletta (1)

(1) University of Heidelberg

The latest LIGO-Virgo-KAGRA observational run has narrowed the local binary black hole merger rate to 14-26 $Gpc^{-3}yr^{-1}$. Despite the increasing number of observations, current state-of-the-art binary population synthesis codes tend to overestimate this rate, revealing a tension between theoretical models and gravitational wave data.
In this talk, I identify and discuss the primary drivers of this discrepancy. A key factor shaping binary black hole merger rates is the metal-dependent star formation rate, as metallicity plays a crucial role in the evolution and fate of massive stars. I will demonstrate that the over-prediction cannot be reconciled solely by adjusting the metal-dependent star formation rate history. Instead, the tension points toward gaps in our understanding of binary evolution.
I will provide a systematic review of the binary evolution uncertainties at play, focusing on the main ingredients that can alleviate this tension, from the common envelope evolution physics and physics of mass transfer, to the natal kicks. Finally, recent observations of dormant black holes by Gaia provide further insights into the formation channels of black hole binaries. I will explore how these data can complement gravitational wave observations and help shed light on the formation and evolution of merging binary black holes.

375	**Geon Propagator in Causal Dynamical Triangulations**	Johannes Anzengruber	Contributed talk (16:40-17:00)

Axel Torsten Maas (1) Simon Platzer (1) Johannes Anzengruber (1)

(1) University of Graz

As with gauge theories in flat-space, physical observables in quantum gravity have to be constructed from gauge invariant correlation functions. An analysis of curvature-curvature correlation functions at time-oriented distances within causal dynamical triangulations, a lattice theory of quantum gravity, shows a behaviour consistent with a massive particle-like state. Hinting at the existence of a geon, a state of self-bound gravitons, the results presented could also have implications for dark matter emerging from pure gravity.

673	**Impact of quantum gravity on the UV sensitivity of extremal black holes**	Francesco Ferrarin	Invited talk (17:00-17:20)

Francesco Del Porro (1) Francesco Ferrarin (1) Alessia Platania (1)

(1) University of Copenhagen, Niels Bohr Institute

Recent work has revealed that extremal Kerr black holes may exhibit a sensitivity to higher-derivative corrections to Einstein's equations, displaying singularities in the tidal forces at the horizon. However, in a purely gravitational context, this "ultraviolet sensitivity" translates into a strong dependence on the Wilson coefficients in the low-energy effective field theory. These, in turn, are fixed by the underlying theory of quantum gravity in the ultraviolet. We find a prediction for these coefficients within the framework of asymptotically safe quantum gravity, and show that, if the quantum gravity scale is trans-Planckian, this horizon-scale ultraviolet sensitivity is avoided.

	Discussion		(40 min.)

M40 - Phenomenology and Novel Observables at Future Colliders

M40 – Session 1 (Wed 23, 16:00-18:00)			
ID	Title	Speaker	Type
555	**Getting the most from the Higgs boson**	Freya Blekman	Invited talk (16:00-16:30)

Freya Blekman (1)

(1) DESY & University of Hamburg, Germany

Particle physics is at a tipping point after the discovery of the Higgs boson in 2012. Investigating the only ever observed spin-zero fundamental particle is of the highest priority and will take many years. A detailed study of the Higgs boson is linked to solutions to some of the burning open questions in particle physics today, while other big questions the LHC was designed to address remain unanswered. At the same time, particle physics relies on large-scale infrastructure that requires extremely long-term planning and commitment.
This means timelines and related questions are also on the minds of particle physicists: what will particle physics be like in 2030, 2040 or 2050? Or more specifically, what are the big questions that can be answered in particle physics in the near future, what are the longer-term challenges, and how urgent is the need for new accelerator facilities, and the pros (and cons!) of these important choices that will need to be made soon. The presentation is intended for a general physics audience.

554	**Novel computational methods for the interpretation of collision data**	Michael Spannowsky	Invited talk (16:30-17:00)

Michael Spannowsky (1)

(1) KIT, Karlsruhe, Germany

Modern collider experiments produce increasingly complex and information-rich data sets, calling for new computational strategies for their interpretation. In this talk, I will discuss recent developments in data analysis methods aimed at improving the extraction of physical information from collision events, with an emphasis on machine learning, quantum machine learning, and related statistical techniques. These approaches open new possibilities for precision studies, classification, anomaly detection, uncertainty-aware inference, and the efficient use of high-dimensional event information. I will highlight how such methods can complement more traditional analysis strategies and help address both practical and conceptual challenges in the interpretation of current and future collider data. The focus will be on general ideas and emerging directions that connect advanced computation with fundamental questions in particle physics.

767	**Simulation of High Energy Physics at Future Colliders**	Simon Plätzer	Contributed talk (17:00-17:15)

Simon Plätzer (1)

(1) Universität Siegen

The simulation of high energy particle reactions is central to the design and interpretation of current and future particle collider experiments. In this talk I will present the state of the art of such event generator simulations, and the significant challenges posed by future experiments and analysis techniques. A novel role is played by the quest for a detailed understanding of final states at the level of individual hadronic final state particles, and many techniques which are now entering the theoretical basis and computational paradigms of these simulations share similarities with many-body physics and open quantum systems.

733	**Subleading Higgs effects at lepton colliders**	Duifje van Egmond	Contributed talk (17:15-17:30)

Duifje van Egmond (1)

(1) ICTP-SAIFR, Sao Paulo

The description of the Higgs mechanism as a spontaneous breaking of gauge symmetry has been hugely successfull in describing the electroweak sector. Despite this success, it is theoretically inconsistent and leads to explicit gauge dependence beyond the mass determination. The Frohlich-Morchio-Strocchi (FMS) framework maintains the successfull mass determination of the textbook Higgs mechanism, while providing a consistent picture for e.g. spectral density functions. In this talk I will discuss how, following the FMS construction, subleading Higgs effects will come into play which could be detectable in (near) future colliders.

49	**FMS on the lattice -- the structure of asymptotic states in weak physics**	Georg Wieland	Contributed talk (17:30-17:45)

Patrick Jenny (1) Axel Torsten Maas (1) Sofie Martins (1) Georg Wieland (1)

(1) University of Graz

Gauge invariance requires physical states to be composite, even in the weak sector of the Standard Model (SM). The Fröhlich-Morchio-Strocchi (FMS) mechanism resolves this subtlety and predicts additional Higgs contributions in SM processes. In this talk, we explore the FMS mechanism on the lattice by simulating a proxy theory with vectorial leptons. We investigate the physical spectrum of this theory non-perturbatively and examine PDFs as well as cross sections, taking a closer look at the internal structure of the composite Higgs and W/Z bosons, and searching for deviations from standard phenomenology.

M41 - Hybrid Intelligence for the Quantum Era

M41 – Session 1 (Fri 25, 10:30-12:30)			
ID	Title	Speaker	Type
806	**Emerging topics in neuromorphic photonic systems**	Sina Saravi	Invited talk (10:30-11:00)

Sina Saravi (1)

(1) Heinz Nixdorf Institute, Paderborn University, Germany

Neuromorphic photonic systems are emerging as an attractive platform for realization of artificial intelligence (AI) computational systems that run on light. Their potential for low-energy-consuming computations and high-capacity information processing, makes them a promising alternative or complementary solution to the conventional electronic-based systems. In this talk, I will present an introduction into the operation principles of neuromorphic photonic systems, followed by an overview of some of the existing and emerging research directions in this field.

807	**Hybrid nanoprinted neural networks: From passive optical inference to engineered photonic computing**	Elena Goi	Invited talk (11:00-11:30)

Elena Goi (1)

(1) Institute of Applied Physics, Abbe Center of Photonics, Friedrich Schiller University Jena, Albert-Einstein-Straße 15, 07745 Jena, Germany

Diffractive neural networks (DNNs) exploit the nature of light propagation in free space and the interaction of a light field with metasurfaces designed with machine learning (ML) methods to implement inference passively in the optical domain1. In this way, DNNs can achieve all-optical ML tasks such as image classification, image compression or decryption2. When fabricated with two photon nanolithography (TPN) methods, DNNs can express their full potential achieving a neuron density of >500 million neurons per square centimeter, operative wavelength in the near infrared or visible wavelength regime and on-chip integration with imaging sensors, such as commercial complementary metal-oxide-semiconductor (CMOS) sensors3. This co-integration is particularly relevant because fully passive nanoprinted DNNs also have intrinsic limitations. Their performance can be highly sensitive to printing errors, alignment tolerances, optical aberrations, and deviations between the simulated and fabricated structures4. After fabrication, the diffractive elements are static and cannot easily be reconfigured or tuned. Moreover, the implementation of hidden optical nonlinearities remains challenging, although nonlinearity is essential for solving more complex ML tasks. Additional limitations arise from the training process itself: many current models rely on approximate scalar diffraction physics, simplified material descriptions, and limited treatments of nanophotonic effects, fabrication constraints, and energy efficiency. Hybrid optoelectronic architectures offer a practical route to overcome part of these limitations. In these systems, the nanoprinted DNN performs large-scale optical transformations and information compression, while the CMOS sensor provides optoelectronic conversion and a nonlinear digital interface that can be modelled, in first approximation, as a shifted ReLU activation. The digitized output can then be processed by a compact electronic neural network. For selected tasks, such hybrid optoelectronic neural networks can reach performances comparable to purely digital networks while substantially reducing the computational load required in the digital domain. In this talk, I will discuss both the potential and the current bottlenecks of nanoprinted DNNs, including fabrication-error sensitivity, static operation, nonlinear activation, training strategies, approximate physical modelling, limited nanophotonic design frameworks, and alignment constraints. I will then present several directions from our work aimed at addressing these challenges, including the development of energy-aware hierarchical optimization strategies for DNNs, the study of optical nonlinearity as a physical computational resource and the exploration of analog photonic computing with engineered materials. Together, these approaches point toward a broader framework in which nanoprinted optical neural networks are not treated simply as passive phase masks, but as physically engineered photonic computing platforms.

1. Lin, X. et al. All-optical machine learning using diffractive deep neural networks. Science 361, 1004–1008 (2018).
2. Goi, E. et al. Nanoprinted high-neuron-density optical linear perceptrons performing near-infrared inference on a CMOS chip. Light Sci. Appl. 10, 40 (2021).
3. Goi, E., Schoenhardt, S. & Gu, M. Direct retrieval of Zernike-based pupil functions using integrated diffractive deep neural networks. Nat. Commun. 13, 7531 (2022).
4. Chen, M., Schoenhardt, S., Gu, M. & Goi, E. Quantitative comparison of the computational complexity of optical, digital and hybrid neural network architectures for image classification tasks. Opt Express 31, 44474–44485 (2023).

M42 - Advances in Magnonics

M42 – Session 1 (Thu 24, 10:30-12:45, Chair: Dieter Süss) Magnonic Crystals, Nanostructures & Collective Phenomena			
ID	Title	Speaker	Type
173	**Dancing Magnets: Reconfigurable Spin Dynamics in Artificial Spin Lattices**	Benjamin Jungfleisch	Invited talk (10:30-11:00)

Benjamin Jungfleisch (1,2)

(1) TU Graz
(2) University of Delaware

Artificial spin systems composed of interacting nanomagnets provide a model platform to investigate collective phenomena in designed magnetic lattices. In these systems, magnetic microstates can be mapped onto effective spin-lattice models, enabling direct experimental access to frustration, degeneracy, and emergent behavior in complex energy landscapes [1].
Beyond their static properties, these systems host a rich spectrum of spin-wave excitations that are strongly determined by the underlying magnetic configuration and lattice geometry [2–5]. They therefore offer a unique opportunity to explore how interactions, symmetry, and microstate selection influence the dynamical response of correlated spin systems. In addition to the fundamental phenomena they exhibit, these systems are also promising for applications in reservoir computing and unconventional computing paradigms [6].
In this talk, I will demonstrate how the excitation spectrum of strongly interacting nanomagnetic arrays can be tailored through the interplay of material properties, lattice design, and reconfigurable magnetic states [7]. These results establish artificial spin systems as a versatile platform for studying and engineering collective excitations in complex magnetic matter.

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[2] S. Lendinez, M. T. Kaffash, and M. B. Jungfleisch, Nano Lett. 21, 1921 (2021).
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[4] R. Sultana, M. T. Kaffash, G. Gubbiotti, Y. Ji, M. B. Jungfleisch, and F. Montoncello, ACS Appl. Electron. Mater. 8, 482 (2026).
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[7] R. Sultana, A. K. Mondal, V. S. Bhat, K. Stenning, Y. Li, D. M. Arroo, A. Vasdev, M. R. McCarter, L. E. De Long, J. T. Hastings, J. C. Gartside, and M. B. Jungfleisch, J. Appl. Phys. 138, 061101 (2025).

228	**Hybrid nanostructures for on-chip excitation of ultrashort wavelength magnons**	Dirk Grundler	Invited talk (11:00-11:30)

Dirk Grundler (1) Anna Duvakina (1)

(1) EPFL

Nanotechnology in magnonics advanced considerably in recent years and allowed for on-chip excitation of coherent magnons with wavelengths down to about 50 nm [1]. Still further progress is needed to optimize the performance of magnons in integrated circuits. We explore two routes to advance nanomagnonics and enhance the frequency bandwidth of on-chip excited magnons. On the insulating ferrimagnet yttrium iron garnet (YIG) we integrated metallic nanodisks which we irradiated by microwave-modulated laser light to excite their plasmonic resonance. Using inelastic light scattering (BLS) microscopy we evidenced the emission of short-wave magnons in YIG [2]. Stimulated by magnon band structure modifications by surface corrugation [3] we deposited ferromagnetic thin films of metallic Ni80Fe20 on specific periodic lattices of DNA nanostructures with feature sizes (lattice periods) on the nm (10 nm) length scale. Spatially resolved x-ray magnetic circular dichroism and BLS measurements indicated the local modification of static and dynamic Ni80Fe20 properties, respectively, by the DNA. In our talk, we report on our recent experiments in nanomagnonics. We thank SNSF for financial support via grant No. 197360 and the following collaborators for their cooperation: V. Karakhanyan, M. Xu, M.A. Suarez, A.J.M. Deenen, M. Raschetti, A. Mucchietto, T. Grosjean, S. Wintz, M. Pascal, and M.M.C. Bastings.

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238	**Perspectives on inverse-design magnonics**	Franz Vilsmeier	Invited talk (11:30-12:00)

Franz Vilsmeier (1) Claas Abert (1) Florian Bruckner (1) Andrii V. Chumak (1) Dieter Suess (1)

(1) University of Vienna

Magnonic devices exploit spin waves - the collective excitations of ordered magnets - for wave-based information processing without charge flow. Their performance hinges on a high-dimensional design space spanning geometry, local material parameters, magnetic field landscape, excitation, and nonlinearity, much of which is inaccessible to manual parameter studies.
Inverse design reverses the conventional workflow: the desired functionality is specified as an objective, and an algorithm finds the optimal structure automatically. The field has advanced rapidly since its founding works in 2021 [Wang et al., Nat. Commun 12, 2636 (2021); Papp et al., Nat. Commun. 12, 6422 (2021)], encompassing topology optimisation of magnonic demultiplexers and filters, ion-irradiation-based gradient-index lenses, experimentally realised reconfigurable radio-frequency devices and Boolean logic gates, and the development of dedicated differentiable micromagnetic solvers that bring the infrastructure of machine learning to the Landau-Lifshitz-Gilbert equation.
In this talk, I give an overview of inverse-design magnonics, organising the emerging literature along two axes - the design degrees of freedom that can be optimised, and the algorithmic toolbox available to do so - and lay out the principal bottlenecks that currently constrain the field. Building on this, I outline what I view as the most promising open frontiers - such as input shaping, nonlinear design and integrated amplification - with the long-term vision of a universal, software-defined magnonic device.

685	**Magnon Kerr effect in ferrimagnetic thin films**	Davit Petrosyan	Contributed talk (12.00-12:15)

Davit Petrosyan (1) Hiroki Matsumoto (1,2) Hanchen Wang (1) Jamal Ben Youssef (3) Richard Schlitz (4) William Legrand (1,5) Pietro Gambardella (1)

(1) Department of Materials, ETH Zurich, CH-8093 Zurich, Switzerland
(2) Institute for Chemical Research, Kyoto University, 6110011 Uji, Japan
(3) LabSTICC, CNRS, Université de Bretagne Occidentale, 29238 Brest, France
(4) Department of Physics, University of Konstanz, 78457 Konstanz, Germany
(5) Université Grenoble Alpes, CNRS, Institut Néel, 38042 Grenoble, France

Cavity magnonics studies the coherent interaction between magnons and microwave photons, providing a platform to explore light-matter interaction in magnetic materials [1]. Driving the system into the nonlinear regime unlocks new magnonic phenomena, such as power-dependent frequency shifts [2] and bistability of magnons [3]. Among magnon nonlinearities, the magnon Kerr effect (MKE) appears universally in ferromagnetic systems with finite anisotropy and manifests as a self-induced frequency shift of the magnon modes. We have studied the MKE using a high-quality 200-nm thick yttrium iron garnet film, grown by liquid phase epitaxy, in a strongly coupled magnon–photon system [4]. The cavity is of the loop-gap type, optimized to couple with thin films of magnetic insulators [5]. The MKE is probed as frequency shifts of the magnon–polariton branches when increasing the microwave power, and the cavity serves as a sensitive probe of the magnon dynamics. We investigate the MKE for all orientations of the magnetization with respect to the film plane. The experimental data is well described by a newly derived theoretical model of the MKE in a thin ferromagnetic film [6]. Our study predicts the trade-off between anharmonicity of a magnonic system and the threshold for coherent magnon–photon coupling, which is necessary to probe the magnetization dynamics.

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337	**Nanoscale YIG Magnonic Crystals: One- and Two-Dimensional Systems**	Khrystyna Levchenko	Contributed talk (12:15-12:30)

Khrystyna Levchenko (1) Kristýna Davídková (1) Mathieu Moalic (2) Rostyslav Serha (1) Carsten Dubs (3) Michal Urbánek (4) Maciej Krawczyk (2) Andrii Chumak (1)

(1) Faculty of Physics, University of Vienna, Austria
(2) Department of Physics of Nanostructures, Adam Mickiewicz University, Poznań, Poland
(3) INNOVENT e. V. Technologieentwicklung, Jena, Germany
(4) CEITEC Nano, Brno University of Technology, Czech Republic

Magnonic crystals (MCs) with nanoscale periodic modulation enable control of spin-wave (SW) band structures for radio-frequency (RF) signal processing. While one-dimensional (1D) MCs provide frequency-selective transmission via Bragg scattering, extending periodicity to two dimensions (2D) enables more flexible band-structure engineering and controlled SW routing.
Here, we realise nanoscale 1D MCs based on 100 nm-thick yttrium iron garnet (YIG) nanowaveguides patterned with periodic nanoholes. Spin-wave propagation over distances exceeding 5 μm is demonstrated using propagating spin-wave spectroscopy (PSWS) and micro-focused Brillouin light scattering (μ-BLS) in the Damon–Eshbach geometry. Transmission and rejection bands appear in the 7.5–10.5 GHz range, with up to six band gaps and signal suppression reaching 26 dB, confirming strong Bragg reflection. Nanoscale confinement yields sharp band edges and reduced multimode contributions. Micromagnetic simulations reproduce the band structure and reveal two anticrossings at 3.1 and 18.7 rad/μm, with single-mode operation below the first anticrossing.
Extending to 2D MCs lithographically realised as planar antidot lattices from 100 nm-thick YIG films, we investigate SW propagation using PSWS and μ-BLS in the in-plane geometries. Defect-free and engineered-defect configurations enable increased functional density and controlled SW routing through defined defect channels, providing a basis for advanced magnonic systems, including topological MCs [6] and three-dimensional magnonic nanocrystals.

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589	**Magnon quantum geometry in one-dimensional chiral magnets**	Sidhartha Chatterjee	Contributed talk (12:30-12:45)

Sidhartha Chatterjee (1) Andreas Haller (1) Thomas L. Schmidt (1) Peter P. Orth (2)

(1) University of Luxembourg
(2) Saarland University

We develop a theoretical framework for magnon dynamics in a quasi-one-dimensional Heisenberg spin chain that includes a nearest-neighbour Dzyaloshinskii-Moriya interaction (DMI) and a magnetic field applied along both the hard and easy axes. Depending on the field's direction and strength, the system hosts various ground states, including ferromagnetic and conical spiral phases, as well as a chiral soliton lattice. Using the Holstein-Primakoff transformation, we derive a quadratic magnon Hamiltonian. We diagonalize the Hamiltonian via the Bogoliubov transformation and show that the quantum geometric tensor of magnons fundamentally inherits a symplectic structure. This geometric structure yields corrections to the semiclassical equations of motion for magnon wave packets, resulting in a metric-driven longitudinal contribution in one dimension. The nonlinear soliton texture also induces non-trivial flat bands and magnon localization. Overall, the framework provides a systematic route for incorporating geometric effects and symplectic structure into magnon dynamics, where no particle-number-conserving framework exists, offering new insights into the interplay between topology and transport in nonlinear spin textures.

M42 – Session 2 (Thu 24, 16:00-18:00, Chair: Andrii Chumak) Quantum Magnonics, Cryogenic & Strong-Coupling Phenomena			
ID	Title	Speaker	Type
721	**Dynamical Stabilization of Inverted Magnetization and Antimagnons by Spin Injection in BiYIG**	Pietro Gambardella	Invited talk (16:00-16:30)

Pietro Gambardella (1)

(1) ETH Zurich

Dynamical stabilization of nonequilibrium energy states is a topic of broad relevance to physics, mechanics, and biology. Dynamical stabilization can be achieved by coupling a system to a nonthermal bath, inducing a phase transition that drives the system out of its ground state and stabilizes a high-energy stationary state. These so-called dissipative phase transitions are much less studied than traditional ones driven, e.g., by temperature or applied fields. However, they are attracting increasing interest because they provide access to unusual states of matter, in which fluctuations of the order parameter change character across the transition, leading to drastic changes in the dynamical response function of the system. The magnetic analogue of a dissipative phase transition consists in switching the magnetization against an external field, dynamically stabilizing a uniform magnetic state with negative energy magnon excitations, so-called antimagnons. Here we use current-induced spin-orbit torques that enable spin injection across a macroscopic sample to induce dynamic stabilization of the magnetization in a Bi:YIG layer combining exceptionally low damping with nearly-compensated magnetic anisotropy [1]. This allows us to tune dissipation to the level required to reach the symmetry-breaking steady state without "killing" the nonequilibrium dynamics via positive damping. Magneto-optical Kerr effect measurements and micromagnetic simulations provide clear signatures of a dissipative phase transition leading to full inversion of the spin population, elucidating the role of nonlinear magnon scattering, magnetic field, and system's size in dynamical stabilization of the magnetization.

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325	**Identifying Loss Contributions in Spin-Wave Transducers**	Florian Bruckner	Invited talk (11:00-11:30)

Florian Bruckner (1) Claas Abert (1) Andrii V. Chumak (1) Kristýna Davídková (1) Iason-Konstantinos Douveas (1) Dieter Suess (1)

(1) Faculty of Physics, University of Vienna, Austria

Spin-wave-based signal processing devices are promising candidates for compact, energy-efficient components in future 5G systems, including delay lines [1] and power limiters [2]. However, further optimization requires a detailed understanding of where energy is lost during transduction and propagation.
In this work, we present a systematic approach to identifying and quantifying individual loss contributions in spin-wave transducer systems. We combine micromagnetic simulations [3] with experimental S-parameter measurements to decompose the total insertion loss into its constituent parts: reflection losses from impedance mismatch, ohmic losses in the transducer metallization, propagation losses due to magnetic damping, and directional losses from spin-wave emission opposite to the intended direction. Each contribution is extracted independently from the measured impedance matrix, enabling a direct comparison between predicted and observed total transmission.
Our analysis reveals that for typical geometries at short spin-wave wavelengths, ohmic losses represent the dominant loss mechanism, while reflection losses can be addressed through impedance matching by scaling the transducer length. Simulations show that the transducer impedance scales approximately linearly with length, allowing prediction of the
optimal geometry from a single reference measurement. We explore strategies to reduce ohmic losses, including modifications to transducer thickness and operation at longer wavelengths. Applying the loss separation to experimental data from YIG-based devices, we identify residual discrepancies between model predictions and measured losses, pointing toward additional loss channels not yet captured and guiding further optimization.

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377	**Three-Dimensional Magnonics: From Coherent Excitation to Transport Perspectives**	Huixin Guo	Contributed talk (17:00-17:15)

Amalio Fernandez-Pacheco (1) Takeaki Gokita (1) Mateusz Gołębiewski (2) Dirk Grundler (3) Huixin Guo (1) Jakub Jurczyk (1) Maciej Krawczyk (2) Kilian Lenz (4) Jürgen Lindner (4) Ryszard Narkowicz (4) Mingran Xu (5) Le Zhao (1)

(1) TU Wien
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Three-dimensional (3D) magnonics is emerging as a promising direction for extending wave-based information processing beyond planar device concepts. 3D magnetic architectures open opportunities for tailoring high-frequency dynamics and guiding microwave signals in all three spatial directions on a chip. Yet, achieving coherent excitation and reliable readout in fully connected 3D nanomagnetic systems remains a central challenge.
Here I present recent progress based on a scalable nanofabrication route combining two-photon lithography and atomic layer deposition. Using this approach, we realized fully connected 3D ferromagnetic Ni woodpile nanonetworks and observed rich spin-wave spectra with distinct bulk and surface modes up to 25 GHz. To coherently access these modes, we developed two complementary device platforms. In a narrowband approach, entire 3D crystals were embedded in a planar microwave microresonator and studied by ferromagnetic resonance at discrete frequencies. In a broadband approach, the crystals were integrated onto a coplanar waveguide, while micro-focused Brillouin light scattering enabled spatially resolved detection on selected structural levels. Together, these approaches establish pathways for coherent spectroscopy of 3D magnonic crystals. I will also discuss the next step toward 3D magnon transport and reconfigurable functionality, where spin-wave transmission is expected to depend sensitively on magnetic states. Realizing such functionality requires fabrication approaches with enhanced geometrical control and material flexibility. In this context, I will outline ongoing work at TU Wien based on focused electron beam induced deposition of 3D ferromagnetic nanostructures, which offers high-resolution direct-write fabrication, smaller feature sizes, and access to Fe-based architectures. First fabricated structures and initial magnetic characterization pave the way toward future studies of state-dependent magnon transport in 3D magnetic conduits.

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669	**Advances in micro-BLS: forward volume spin waves and polarization-dependent measurements**	Krzysztof Szulc	Contributed talk (17:15-17:30)

Krzysztof Szulc (1) Mengying Guo (2) Xiufeng Han (3) Jan Klima (1) Jakub Krčma (4) Dominik Pavelka (1) Michal Urbánek (1) Hongyu Wang (3) Qi Wang (2) Ondřej Wojewoda (5)

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Micro-focused Brillouin light scattering (BLS) spectroscopy is one of the most versatile methods to probe spin-wave dynamics. Typically, magnons are measured by detecting scattered light whose polarization is rotated by 90° relative to the incident beam. However, this conventional approach assumes the presence of only linear magneto-optical coupling. Generally, this assumption is not true, especially in magnetic garnets, where the contribution of the quadratic magneto-optical effect can be significant.
In this study, performed on coherently excited spin waves in a 100 nm-thick bismuth-doped yttrium iron garnet (BiYIG) thin film, we systematically analyzed the polarization dependence of the BLS signal by modifying the angle of both the polarizer and analyzer [1]. By sweeping their angles, we obtained polarization-dependent spectra for all basic spin-wave geometries: backward volume, Damon–Eshbach, and forward volume. To interpret the measurements, we employed a semi-analytical model that combines calculated electric-field distributions with spin-wave dispersion and dynamic magneto-optical susceptibility including both linear (Kerr) and quadratic (Cotton–Mouton) contributions. Fitting the experimental data reveals that the Cotton–Mouton effect in BiYIG is comparable in magnitude to the linear Kerr effect, highlighting the importance of nonlinear contributions in accurately describing magneto-optical interactions.
Furthermore, we resolved the dispute about the feasibility of measuring the forward volume spin waves in BLS. We demonstrated that a high numerical aperture objective significantly modifies the local electric field, introducing non-negligible out-of-plane and transverse components even for nominally linearly polarized input light. This field redistribution enables sensitivity to all components of dynamic magnetization, making micro-focused BLS measurements in the forward volume geometry possible.

[1] K. Szulc et al. arXiv:2602.15760 (2026).

338	**Ultralong-Living Magnons in the Quantum Limit**	Rostyslav Serha	Contributed talk (17:30-17:45)

Rostyslav Serha (1) Kaitlin McAllister (2) Fabian Majcen (1) Sebastian Knauer (1) Timmy Reimann (3) Carsten Dubs (3) Genadiy Melkov (4) Alexander Serga (5) Vasyl Tyberkevych (6) Andrii V. Chumak (1) Dmytro Bozhko (2)

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(6) Oakland University, Rochester, USA

Quantum magnonics explores magnons—quasiparticles of spin waves—as carriers of quantum information, enabling coherent coupling to superconducting qubits and single-magnon detection [1,2]. Yttrium iron garnet (YIG) remains the material of choice due to its exceptionally low magnetic damping; however, magnon lifetimes at GHz frequencies are typically limited to ~1 μs for the uniform ferromagnetic resonance mode, constraining coherent quantum applications [3]. Here, we demonstrate record-long magnon lifetimes in the quantum limit ($T \to 0$), exceeding 18 μs at 1.6 GHz for short-wavelength dipolar-exchange magnons in an ultra-pure single-crystal YIG sphere at millikelvin temperatures [4]. Lifetimes were extracted using broadband ferromagnetic resonance spectroscopy combined with measurements of the three-magnon parametric instability threshold, giving direct access to short-wavelength magnon relaxation rates inaccessible by conventional means. The results reveal strong suppression of multi-magnon and magnon–phonon scattering in the quantum regime. Compared to the uniform mode, short-wavelength magnons exhibit reduced sensitivity to surface defects and lattice imperfections, enabling substantially longer lifetimes. At the lowest temperatures, all extrinsic relaxation channels are frozen out, and the lifetime becomes governed solely by intrinsic material purity. The observed 18 μs lifetime sets a new benchmark for magnetic coherence, placing magnons on a timescale comparable to superconducting qubits and opening a pathway toward hybrid solid-state quantum networks [3].

[1] D. Lachance-Quirion, S. P. Wolski, Y. Tabuchi, et al., Science 367, 425 (2020).
[2] D. Xu, X.-K. Gu, H.-K. Li, et al., Phys. Rev. Lett. 130, 193603 (2023).
[3] R. O. Serha, C. Dubs, A. V. Chumak, APL Materials 14, 030401 (2026).
[4] R. O. Serha, K. H. McAllister, F. Majcen, et al., arXiv:2505.22773 (2025).

732	**Strong magnon-spin coupling and size effects on Van-der-Waals antiferromagnet CrSBr**	David Garcia Pons	Contributed talk (17:45-18:00)

David García Pons (1) Jorge Pérez-Bailón (1) Carla Boix-Constant (2) Iván Gómez-Muñoz (2) Xavier del Arco-Fargas (1) Samuel Mañas-Valero (2) Eugenio Coronado (2) David Zueco (1) María-José Martínez-Pérez (1)

(1) Instituto de Nanociencia y Materiales de Araqón (CSIC - Universidad de Zaragoza)
(2) Instituto de Ciencia Molecular (ICMOL)

Cavity Quantum Electrodynamics (C-QED) is used to manipulate and interrogate qubits or to engineer hybrid light-matter states. However, cavity photons impose severe restrictions on their maximum coupling strength to paramagnetic objects, thus limiting the accessible regimes and the physics that can be explored in C-QED platforms. Beyond light, the solid state offers different quantized bosonic excitations, such as magnons, the quantum of spin waves in magnetic solids. The rich physics of light-matter hybrids is, in principle, also applicable to magnon-matter states, which come with additional advantages such as reduced size and enhanced coupling strengths.

Here we report on magnon-spin interaction between the layered van der Waals antiferromagnet CrSBr [1,2] and paramagnetic ion crystal GdW10 [3], measured via microwave absorption spectroscopy at millikelvin temperatures. The avoided crossing found at low probing power [4] indicates we achieve the strong coupling regime of interaction between both systems, while higher probing power saturates the paramagnet, thus losing the anticrossing. This result opens a path for the use of CrSBr and similar layered materials as magnonic platforms in hybrid quantum systems, both for fundamental physics and device-oriented experiments.
Complementing these results, we performed measurements of microscopic CrSBr flakes integrated on chip, which give us insights into controlling dispersion and thus linewidth of the magnonic modes, bringing us closer to integrating Van der Waals antiferromagnets into functional devices.

[1] Nano Letters 2022 22 (16), 6716-6723
[2] Nano Letters 2024 24 (15), 4319–4329
[3] Physical Review Letters 2012 108, 247213
[4] arXiv:2508.17888

M42 – Session 3 (Fri 25, 10:30-12:30, Chair: Benjamin Jungfleisch) Spin-Wave Devices, Transducers & Inverse Design,

ID	Title	Speaker	Type
799	**Patterning two-dimensional gradients in structural and magnetic properties for spintronics and magnonics applications**	Ales Hrabec	Invited talk (10:30-11:00)

Ales Hrabec (1,2)

(1) Laboratory for Mesoscopic Systems, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland
(2) PSI Center for Neutron and Muon Sciences, 5232 Villigen PSI, Switzerland

Novel spin-based logic architectures are being developed to provide high-performance nonvolatile data retention and processing. Two prominent directions include the development of spin-based in-memory computing and efficient, all-electric control of magnetic order. We have recently showed that spatial patterning of uniaxial anisotropy via selective oxidation can result in strong lateral coupling based on the Dzyaloshinskii–Moriya interaction [1]. The coupling can be incorporated into electrically-controlled devices comprising reconfigurable NAND and NOR logic gates [2]. Despite the limited number of material systems where such in-memory computing can be realized, the capability of patterning magnetic anisotropy opened unprecedented avenues. This discovery highlighted the need to develop new methods for spatial patterning, which could lead to new, disruptive technologies in magnetism and beyond.
To enhance the pool of structural and magnetic properties that can be patterned, we have developed direct-write laser annealing, which is based on local annealing [3]. Here, the underlying magnetic properties are linked to heat-activated processes such as crystallization, interdiffusion or oxidation. We demonstrate the capability of this technique by realization of a spin wave band pass filter and new architectures for passively resetting the position of a magnetic domain wall [3,4]. We also demonstrate that conventional and unconventional spin-orbit torques can be patterned based on the underlying designed structural gradients in tungsten thin films [5] as well as patterning magnetic properties in thin TmIG films.
The laser annealing-based method opens new opportunities to pattern material and magnetic landscapes with high-precision capability, leading to unprecedented applications in spintronics and magnonics, and thin-film based magnetism in general.

1. Z. Luo et al., Science, 363, 1435 (2019).
2. Z. Luo et al., Nature 579, 214-218 (2020).
3. L. Riddiford, J. A. Brock et al., Nat. Commun. 16, 10979 (2025).
4. J. Brock et al., Nano Lett., 26, 16, 5426–5433 (2026).
5. L. Riddiford, et al., arXiv:2601.01429 (2026).

ID	Title	Speaker	Type
296	**Temperature dependence of volume and interface contributions to the magnetic damping of Permalloy thin films**	Andreas Ney	Invited talk (16:30-17:00)

Fabian Ganss (1) Réne Hübner (1) Kilian Lenz (1) Jürgen Lindner (1) Andreas Ney (2) Verena Ney (2)

(1) Helmholtz-Center Dresden-Rossendorf
(2) Johannes Kepler University

A thorough understanding of magnetic damping in ferromagnetic materials is of importance in spintronics from both a fundamental and a practical point of view. The phenomenological Gilbert parameter α in the Landau-Lifshitz equation is central to quantify the magnetic damping, which can be measured with ferromagnetic resonance (FMR). Permalloy (Py = $Ni_{80}Fe_{20}$) is one of the model systems with low magnetic damping. Here, we report the outcome of a systematic study of the temperature and frequency dependence of the FMR linewidth of Py, which was grown on typical substrates (silicon and sapphire) and capped with materials commonly used for preventing oxidation (Ta, Al, and SiOx). The resulting frequency and temperature dependence of the FMR linewidth deviates significantly from the expected Gilbert-like behavior. Unwanted non-Gilbert-like contributions appear, especially at low temperatures, and particularly for oxidic interfaces [1]. In contrast, metallic capping layers avoid non-Gilbert-like contributions. Special focus was paid to the influence of the Al spacer thickness which was varied between 1 and 10 nm [2]. In particular, Py sandwiched in between a metallic Al cap and a thin spacer layer exhibits negligible inhomogeneous FMR linewidth broadening and a very small, purely Gilbert-like contribution of α = 0.0068(2) down to the lowest temperature for a fixed Py layer thickness of nominally 20 nm [2]. In addition, the Gilbert damping parameter α was studied as a function of Py layer thickness for Al-sandwiched Py thin films. The full FMR dataset allows to separate the Gilbert-like contributions to the FMR linewidth from non-Gilbert-like ones like two magnon scattering processes for the entire thickness series from 3 nm to 37 nm. We can deconvolute α into its respective bulk and interfacial contributions and their respective temperature dependencies. While the bulk contribution monotonously decreases with temperature from 0.0061(1) down to 0.0054(1), and is thus of purely resistivitylike character [3]. In contrast, the interfacial contribution shows a subsequent increase at low temperature, i.e. it contains both resistivity and conductivity-like contributions [3]. The isolated bulk contribution, which is only of resistivity-like character, can be considered to reflect the intrinsic magnetic damping properties of Py thin films.

[1] V. Ney et al. Phys. Rev. Materials 7, 124403 (2023)
[2] V. Ney et al. Phys. Rev. Materials 8, 124410 (2024)
[3] V. Ney et al. Phys. Rev. Materials 10, 024409 (2026)

715	**Probing Spin-wave Nonreciprocity in Ferromagnet/Superconductor Hybrid Structures**	Jan Klima	Contributed talk (11:30-11:45)

Jan Klima (1) Ekaterina Pribytova (2) Jakub Holobrádek (1) Ondřej Wojewoda (3) Krzysztof Szulc (1) Viktor Danchuk (1) Julia Kharlan (4) Jarosław W. Kłos (4) Michal Urbánek (1)

(1) CEITEC Brno University of Technology, Czechia
(2) Brno University of Technology, Czechia
(3) Massachusetts Institute of Technology
(4) ISQI, Adam Mickiewicz University, Poznań, Poland

With quantum computing on the rise, there is an increased need to deal with cryogenic environments, often involving superconducting materials. Hybrid systems utilizing spin waves at cryogenic temperatures could benefit from increased conversion efficiency of electrical and magnonic signals and feature tunable devices, changing their functionality upon crossing the critical temperature of the superconductors involved. The ferromagnet/superconductor (FM/SC) heterostructures also offer enhanced nonreciprocity of the group velocity of Damon–Eshbach spin waves unmatched by other approaches [1,2]. This could be utilized in switchable isolators or non-reciprocal couplers, which are essential components of modern microwave circuits.
Knowledge of the spin-wave dispersion relation is essential for the characterization of spin-wave behavior as well as for the explanation of many magnonic phenomena. In the past years, theoretical models of FM/SC systems have been developed [2, 3], predicting the nonreciprocal upshift in the spin-wave dispersion relation. While there were reports on the frequency upshift [4], the nonreciprocity was yet to be observed.
We will present a variable-gap propagating spin-wave spectroscopy [5] experiment of FM/SC multilayers, determining the spin-wave dispersion relation in a wide frequency and wavevector range, confirming the spin-wave nonreciprocity. The measured dispersion relations compare well to COMSOL simulations and analytical models. The experiments were performed in a 2–300 K temperature range in a commercial cryogenic setup using custom-made high-frequency (0.1–50 GHz) sample holders.

[1] M. Mruczkiewicz and M. Krawczyk, J. Appl. Phys. 115 (2014) 113909
[2] I. A. Golovchanskiy et al., J. Appl. Phys. 124 (2018) 233903
[3] X.H. Zhou et al., Phys. Rev. B 110 (2024) L020404
[4] M. Borst et al., Science 382 (2023) 430–434
[5] M. Vaňatka et al., Phys. Rev. Applied 16 (2021) 054033

394	**Improving the efficiency of antiferromagnetic upconversion**	Verena Brehm	Contributed talk (11:45-12.00)

Verena Brehm (1)

(1) TU Eindhoven

Upconversion is an intriguing process where driving of a low-frequency mode allows the occupation of a higher-frequency mode. We specifically focus on magnonic upconversion in the antiferromagnetic material YFeO3. By strongly pumping the low-frequency (qFM) mode with a laser pulse, the high-frequency (qAFM) mode is populated, as recently demonstrated experimentally [1]. Using a macrospin model, we propose two new ways to make this upconversion process more efficient: (I) By applying a static external magnetic field, and (II) by hybridizing the magnon modes with optical cavity modes.

[1] Zhang et al., Nature Physics 20, 801–806 (2024)

145	**Low Insertion Losses Microscale Spin-wave RF Devices**	Kristyna Davidkova	Contributed talk (12:00-12:15)

Kristýna Davídková (1) Florian Bruckner (1) Iason-Konstantinos Douveas (1) Carsten Dubs (2) Khrystyna Levchenko (1) Dieter Suess (1) Andrii Chumak

(1) Faculty of Physics, University of Vienna, Austria
(2) 2INNOVENT e. V. Technologieentwicklung, 07745, Jena, Germany

The drive toward faster, more efficient 5G communication systems requires radio-frequency (RF) devices to adapt from Frequency Range 1 (FR1, sub 6 GHz) to higher operating frequencies in Frequency Range 2 (FR2, 24.25–71.0 GHz) and the proposed Frequency Range 3 (FR3, 7.125–24.25 GHz). Spin wave (SW) devices are promising candidates, combining efficient operation in the higher frequency range (FR3) with multifunctionality, thereby enabling compact, energy-efficient devices [1]; however, practical adoption is constrained by significant insertion losses [2, 3]. We present a systematic study of insertion losses arising during electromagnetic–spin wave–electromagnetic signal conversion and during SW propagation between a pair of U-shaped transducers in a 1.96 µm thick YIG film. Transducer lengths (60–340 µm) and widths (1–6 µm) are varied to tune impedance matching over a broad frequency range (5–30 GHz). We demonstrate that the insertion loss can be optimized for each operational frequency by selecting the appropriate transducer length. This length defines the spin-wave resistance parameter, which increases as the frequency increases. The lowest measured insertion loss is 6.25 dB at 12 GHz using 200 µm long transducers. Experimental results are compared to micromagnetic simulations [4] to optimize YIG thickness, transducer geometry, and spin wave mode selection.

[1] K. Levchenko, K. Davídková, J. Mikkelsen, and A. Chumak, (2026). Review on spin-wave RF applications. IEEE Transactions on Magnetics.
[2] K. Davídková, K. Levchenko, F. Bruckner et al. (2025). Nanoscale spin-wave frequency-selective limiter for 5G technology. Physical Review Applied 23.3: 034026.
[3] K. Davídková, K. Levchenko, R. Serha et al. (2025). Spin-wave microscale RF delay lines for mid-and high-frequency 5G band. Journal of Applied Physics 138.14.
[4] F. Bruckner, K. Davídková, C. Abert et al. (2025). Micromagnetic simulation and optimization of spin-wave transducers. Scientific Reports 15.1: 19993.

403	**Inverse-design of linear and nonlinear magnonic devices using level-set topology optimization**	Andrey Voronov	Contributed talk (12:15-12:30)

Claas Abert (1) Florian Bruckner (1) Andrii V. Chumak (1) Dieter Suess (1) Andrey Voronov (1)

(1) Faculty of Physics, University of Vienna, Austria

The inverse design approach in magnonics exploits the wave nature of spin waves and machine learning techniques to develop logical devices with functionalities that exceed the capabilities of analytical methods. While promising for analog, Boolean, and neuromorphic computing, current implementations of inverse micromagnetics face significant memory limitations that hinder the design of complex systems. In this work, we present a level-

set parameterization method for topology optimization, combined with an adjoint-state approach for memory-efficient simulation of magnetization dynamics [1]. The framework is implemented in NeuralMag [2], a GPU-accelerated micromagnetic solver featuring a nodal finite-difference scheme and automatic differentiation tools provided by the JAX backend. The level-set method provides a natural way of handling topological changes such as boundary merging, the formation of new shapes, or the disappearance of existing ones, which typically challenge conventional shape optimization approaches. Its combination with the adjoint-state method for solving the Landau-Lifshitz-Gilbert equation enables efficient gradient computation without overwhelming computational resources, thus overcoming the hardware constraints of existing inverse-design algorithms in magnonics.
To validate the method, we designed a 300 nm-wide yttrium iron garnet demultiplexer achieving frequency-selective spin-wave separation, where the gradient-based optimization required fewer simulations compared to the previously used direct binary search method [3]. These results highlight the algorithm's efficiency in exploring local minima across various initial configurations, establishing its utility as a versatile tool for the inverse design of magnonic logic devices. As a next step, we have also achieved the utilization of nonlinear spin-wave behavior within our level-set framework, reproducing the example of a nonlinear switch introduced by Wang et al. [3]. This advancement opens new possibilities for developing complex magnonic logic gates, including half-adders and multi-frequency nonlinear devices, further broadening the applicability of the proposed method for next-generation spintronic technologies.

[1] A. A. Voronov et al., npj Spintronics 3, 19 (2025).
[2] C. Abert et al., npj Computational Materials 11, 1 (2025).
[3] Q. Wang, A. V. Chumak, and P. Pirro, Nat. Commun. 12, 2636 (2021).

M42 – Poster session (PS2 Wed23-Fri25)

ID	Title	Presenter	Type
385 **P079**	**Spin-Wave Transport through S-Shaped Ga:YIG Nanowaveguides**	Hannah Arnfelser	Poster

Hannah Arnfelser (1) Khrystyna Levchenko (1) Franz Vilsmeier (1) Andrey Voronov (1)

(1) Faculty of Physics, University of Vienna, Austria

Spin-wave-based computing has attracted growing interest as a promising approach to overcome fundamental limitations of CMOS technologies, offering low-power operation and inherent wave-based logic functionality. Efficient routing of spin waves through geometrically complex waveguide structures represents a key challenge in realizing integrated magnonic circuits. Ga:YIG has been shown to be a highly suitable material for nanoscale magnonic waveguides (Voronov et al., arXiv:2509.05050, 2025): its strongly reduced saturation magnetization increases the exchange length substantially, pushing propagation into the exchange-dominated regime. This leads to largely isotropic dispersion and noticeably higher group velocities than in non-substituted YIG, making Ga:YIG a natural candidate for spin-wave transport around bends, where conventional in-plane magnetized, dipolar-dominated YIG suffers from strong anisotropy between the Damon-Eshbach (DE) and backward-volume (BV) configurations. Whether such exchange-dominated spin waves can be efficiently transported through geometrically complex structures, involving multiple consecutive bends, remains an open question.
Here, we investigate spin-wave propagation through S-shaped Ga:YIG nanowaveguides consisting of two consecutive 90 bends, where the fixed in-plane external magnetic field combined with the geometry enforces a reorientation of the spin-wave propagation direction relative to the magnetization. BLS measurements reveal spin-wave transmission through both bends in a frequency range of 8.0--8.4\,GHz, with complementary micromagnetic simulations using the finite-element solver Magnum.pi showing qualitative agreement with the measured intensity profiles. Our results suggest that S-shaped Ga:YIG nanowaveguides are promising candidates for spin-wave routing elements in future magnonic networks.

ID	Title	Presenter	Type
480 **P080**	**Optimization of Spin-Wave Transducers via Cross-Validated Simulation, Analytical, and Experimental Methods**	Iason-Konstantinos Douveas	Poster

Iason-Konstantinos Douveas (1) Florian Bruckner (1) Andrii V. Chumak (1) Kristýna Davídková (1) Dieter Suess (1)

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Magnonic devices based on spin-wave (SW) propagation in thin-film yttrium iron garnet (YIG) are promising candidates for compact, low-power RF components targeting 5G frequency bands. A central challenge in their practical adoption is insertion loss, which stems from the transduction of electromagnetic energy into spin waves and back. In this work, we present a comprehensive study of coplanar waveguide (CPW) transducers on YIG thin films, combining micromagnetic simulations performed with magnum.np, analytical modeling based on Kalinikos–Slavin theory, and experiments in a mutually cross-validating framework.
Transducer efficiency is quantified through the spin-wave resistance R_{sw} (which describes the energy put into the spin-wave) and insertion loss. Analytically, R_{sw} is calculated via the Kalinikos–Slavin model. Micromagnetic simulations using magnum.np solve the Landau–Lifshitz–Gilbert equation, incorporating an external bias field and current-induced Oersted fields.
We perform systematic parameter studies — varying conductor width, height, center-to-center spacing, and YIG film thickness — to guide the design of transducers for optimal spin-wave efficiency $\eta_{\mathrm{sw}} = \frac{R_{\mathrm{sw}}}{(R_{\mathrm{sw}}+R_{\Omega})}$ and insertion loss.

ID	Title	Presenter	Type
530 **P081**	**Inverse Design of Coplanar Waveguide Transducers for Directional Spin-Wave Beam Excitation**	Fabian Majcen	Poster

Fabian Majcen (1) Florian Bruckner (1) Andrii Chumak (1) Kristýna Davídková (1) Dieter Suess (1) Franz Vilsmeier (1) Andrey Voronov (1)

(1) Faculty of Physics, University of Vienna, Austria

The field of magnonics, which utilises magnons for energy-efficient data processing, has made significant advances through inverse design. AI-based optimisation is emerging as a powerful tool in such efforts. Prior approaches have optimised the magnetic material itself, through geometry or saturation magnetisation landscapes, as well as reconfigurable scattering media, realising functionalities including RF filtering, logic operations, and neural-network tasks. Inverse design has also been applied to spin-wave excitation waveforms for targeted pulse generation. Here we demonstrate a fundamentally new

approach: inverse-designing the coplanar waveguide transducer geometry. We apply this framework to form directional spin-wave beams, channeling energy without patterned waveguides, thereby reducing fabrication complexity.
The conductor profile is parameterised by piecewise cubic splines through a small set of normalised control points. Fabrication constraints, minimum feature sizes and gap tolerances, are encoded as bounds on these control points, so every candidate geometry explored by the optimiser is intrinsically compatible with lithographic limits. A gradient-based algorithm maximises excitation efficiency at a target wavenumber, sculpting the emission into a defined beam window in the yttrium iron garnet film.
The optimised transducer geometry enables spin-wave beam optics. Beams can be focused, defocused, or steered simply by varying the conductor profile, without additional waveguide patterning. Focused beams concentrate spin-wave intensity, directly lowering the power threshold for nonlinear interactions that drive wave-based computation. Furthermore, a single transducer optimised simultaneously at two frequencies produces two spatially separate beams, realising frequency-demultiplexing directly within the excitation structure.

480 **P082**	**Coherent Microwave Driving of Domain Wall Depinning in a Ferrimagnetic Garnet**	Hanchen Wang	Poster

Hanchen Wang (1) Laura van Schie (1) Adam Erickson (1) Lauren J. Riddiford (1) Davit Petrosyan (1) Christian L. Degen (1) Richard Schlitz (2) William Legrand (3) Pietro Gambardella (1)

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(3) Université Grenoble Alpes

Coherent control of domain wall dynamics offers a route to the fast manipulation of magnetic textures beyond thermally activated motion. We demonstrate the resonant excitation of linear and nonlinear dynamics of a pinned domain wall in a ferrimagnetic garnet thin film driven by a microwave field. Using scanning nitrogen-vacancy magnetometry and nonlocal spin-pumping measurements, we identify a low-frequency mode inside the magnon gap originating from the localized oscillatory motion of a domain wall across a pinning line defined by a Pt stripline. Upon an increase in the microwave drive into the nonlinear regime, this mode enables domain wall depinning at reduced external magnetic fields. Micromagnetic simulations reveal a progression from localized oscillations to partial relocation between pinning sites and ultimately complete escape from the pinning region with increasing driving power. These results establish the resonant excitation of domain walls at engineered pinning sites as a mechanism for manipulating magnetic textures via localized nonlinear dynamics.