JOHANNES KEPLER
UNIVERSITÄT LINZ

73rd Annual Meeting
of the Austrian Physical Society

Johannes Kepler University Linz

23 – 27 September 2024

ÖPG Tagungsband Nr. 73

Linz, 2024

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Divisions of the Austrian Physical Society

ACP	Equal Opportunities in Physics
AKU	Acoustics
AMP	Atoms,Molecules, Quantum Optics and Plasmas
COND	Condensed Matter
ENS	Energy and Sustainability
FAKT	Nuclear Particle Physics
GEP	History of Physics
LHS	Physics and School
MBU	Medical Physics, Biophysics, Environmental Physics
NESY	Research with Neutron and Synchrotron Radiation
OGD	Surfaces, Interfaces and Thin Layers
PIN	Physics Industry
YM	YoungMinds

Contents

We would like to thank our exhibitors and sponsors:

Welcome Address

Dear participants of the 73rd Annual Meeting of the Austrian Physical Society (ÖPG),

on behalf of the entire board of the ÖPG we welcome you to four intense days of scientific presentations, fruitful discussions, and exchange with national and international colleagues.

The conference will start traditionally with the Energy Day, dedicated to the topic “Hydrogen” and organized by the ÖPG division “Energy and Sustainability”. This year, it is our great pleasure to have the Lise Meitner Lecture - jointly organized by the ÖPG and the German Physical Society (DPG) – included in the program. The corresponding talk by Austrian born Astrophysicist Lisa Kaltenegger, Cornell University, USA, on the search for a second earth, will also attract the broad public, including high-school students and their teachers.

Further highlights of the meeting will be the award ceremony, the sessions of the divisions “School and Physics” and “Physics and Industries”, and that of the “Young minds” work group. The session of the “History of Physics” division will include the presentation of 88 year old colleague and Holocaust survivor Peter René Perez, as well as a documentary on the physicist and peace activist Hans Peter Dürr. Also, we are pleased to have this year an attractive session of our reactivated work group “Equality in Physics”.

A novelty will be the Central European Condensed Matter Physics Day, organized by colleagues from Austria, Croatia, Czechia, Hungary, Slovakia, Slovenia, and Switzerland. The meeting will terminate with the public evening talk by last year’s Wittgenstein laureate Hans Briegel, which acts somehow already as an outlook to the 74th annual meeting of the ÖPG, organized together with the Swiss Physical Society (SPG) in the framework of the International Year of Quantum Science and Quantum Technology 2025 at the University of Vienna.

We are looking forward to all together 8 plenary talks, 3 public evening events, several invited talks in the frame of CECMD, Energy Day, SFB BeyondC, the AKCP symposium, as well as 113 contributed talks. From the 34 poster presentations, a jury will select prizes for the best presentations by master and Ph.D. students. Finally, we would like to thank the local organizing committee of the Johannes Kepler University Linz, in particular Andreas Schell and Susanne Schwind.

Christian Teichert, President of ÖPG

Alberta Bonanni, Incoming President of ÖPG

General information about the conference

Conference site and location of rooms

The conference will take place at the campus of the Johannes Kepler University (JKU), mainly in the “Hörsaalgebäude”, “Managementzentrum”, “Bankengebäude” and “Hochschulfondsgebäude”. All the locations relevant for the conference can be found on the map at the end of this book.

Public Transport / Arrival by Car

The campus can be reached via public transport (Linz-Linien) from Linz main train station (Hauptbahnhof) with the tram lines 1 and 2 by exiting at the last stop of these lines "JKU Universität". The Redoutensaal and the Promenadenhof (where the Conference Dinner is taking place) can also be reached with these lines by exiting at "Taubenmarkt".

If you arrive by car, please draw an entrance ticket and pick up your exit ticket (for any duration of stay inside the parking lot or parking house) at the conference desk for a fee of 5 EUR.

Conference website

www.jku.at/oepg2024

Conference Registration

The registration desk for the ÖPG 2024 Conference will be located in the “Raiffeisen Innovation Centre”

Please pick up your name badge, together with the abstract booklet and other information materials at the conference registration desk after your arrival.

Participation Fees:

Category	Member Early Bird	Member Late	Non-Member Early Bird	Late
Regular	€ 150,00	€ 170,00	€ 180,00	€ 200,00
PhD students	€ 100,00	€ 120,00	€ 120,00	€ 140,00
Students before Master/Diploma	€ 60,00	€ 80,00	€ 80,00	€ 100,00
1 day registration	€ 40,00	€ 40,00	€ 40,00	€ 40,00
Conference Dinner	€ 50,00	€ 50,00	€ 50,00	€ 50,00

WiFi / W-LAN Access

You can use Eduroam or pick up your guest account login data at the registration desk.

Lecture Rooms

There will be a laptop and beamer in every lecture room. You can bring your own laptop and/or a USB stick with your presentation.

Poster Session

The Poster Session will be taking place on Tuesday, 24 September, from 14:00 to 15:30 in HS 17 (JKU Business School/Managementzentrum). The pinboards for the placement of posters will be numbered according to the poster number in the program. Poster Size: A0, portrait.

Industrial Exhibition

The industrial exhibition will be taking place from Tuesday, 24/09/2024 to Thursday, 26/09/2024 in front of the lecture halls HS 9 and HS 10 in the Hörsaalgebäude.

Conference Dinner

The conference dinner will be taking place at Promenadenhof Linz (Promenade 39, 4040 Linz) on Wednesday, 25/09/2024 at 7 p.m. The price of 50 EUR includes 2 drinks and has to be paid in advance via the conference registration website **until September 9, 2024**.

Public Lecture by Hans Briegel (University of Innsbruck)

Thursday, 26/09/2024 ,19:00, **Redoutensaal** (Promenade 39, 4040 Linz). Details are yet to be announced.

Lise Meitner Lecture

Monday, 23/09/2024 at 18:30 in HS 10
Lisa Kaltenegger (Cornell University): *Alien Earths: Searching for a Second Earth – Challenges, Opportunities and Adventures*

The detection of exoplanets orbiting other stars has revolutionized our view of the cosmos. First results suggest that it is teeming with a fascinating diversity of rocky planets, including those in the habitable zone. Even our closest star, Proxima Centauri, harbors a small planet in its habitable zone, Proxima b. With JWST and the upcoming Extremely Large Telescopes, we will be able to peer into the atmospheres of rocky planets and get a glimpse into other worlds.

Using our own planet and its wide range of biota as a Rosetta stone, we'll explore how we could detect habitability and signs of life on exoplanets over interstellar distances. The discussion on what makes a planet a habitat and how to detect signs of life is lively. This talk will show the latest results, the challenges of how to identify and characterize such habitable worlds, and how near-future telescopes will revolutionize the field. For the first time in human history, we have developed the technology to detect potential habitable worlds.

Biography

Prof. Lisa Kaltenegger is an award-winning astrophysicist and astrobiologist, Founding Director of the Carl Sagan Institute at Cornell, Professor in Astronomy at Cornell University, and author of Alien Earths: The Science for Planet Hunting in the Cosmos.

Lisa Kaltenegger is a pioneer and world-leading expert in modeling habitable worlds and their light fingerprint and has spent the last decade finding new ways to spot life in the cosmos, working with NASA and ESA from Austria to the Netherlands, Harvard, Germany, and now Cornell. Prof. Kaltenegger is the author of more than 100 peer-reviewed publications.

Among her international awards are the Invited Discourse lecture at the IAU General Assembly in Hawaii, the Heinz Meier Leibnitz Prize for Physics of Germany, the Doppler Prize for Innovation in Science of Austria, and the Barry-Jones Inauguration Award of the Royal Astrobiology Society and Open University in Britain. Her review 2017 on /How to Characterize Habitable Worlds and Signs of Life/ was selected by Annual Reviews as part a collection celebrating pioneering women scientists.

JOHANNES KEPLER UNIVERSITY LINZ

Österreichische Physikalische Gesellschaft

DPG
Deutsche Physikalische Gesellschaft

Alien Earths:
Searching for a Second Earth - Challenges, Opportunities and Adventures

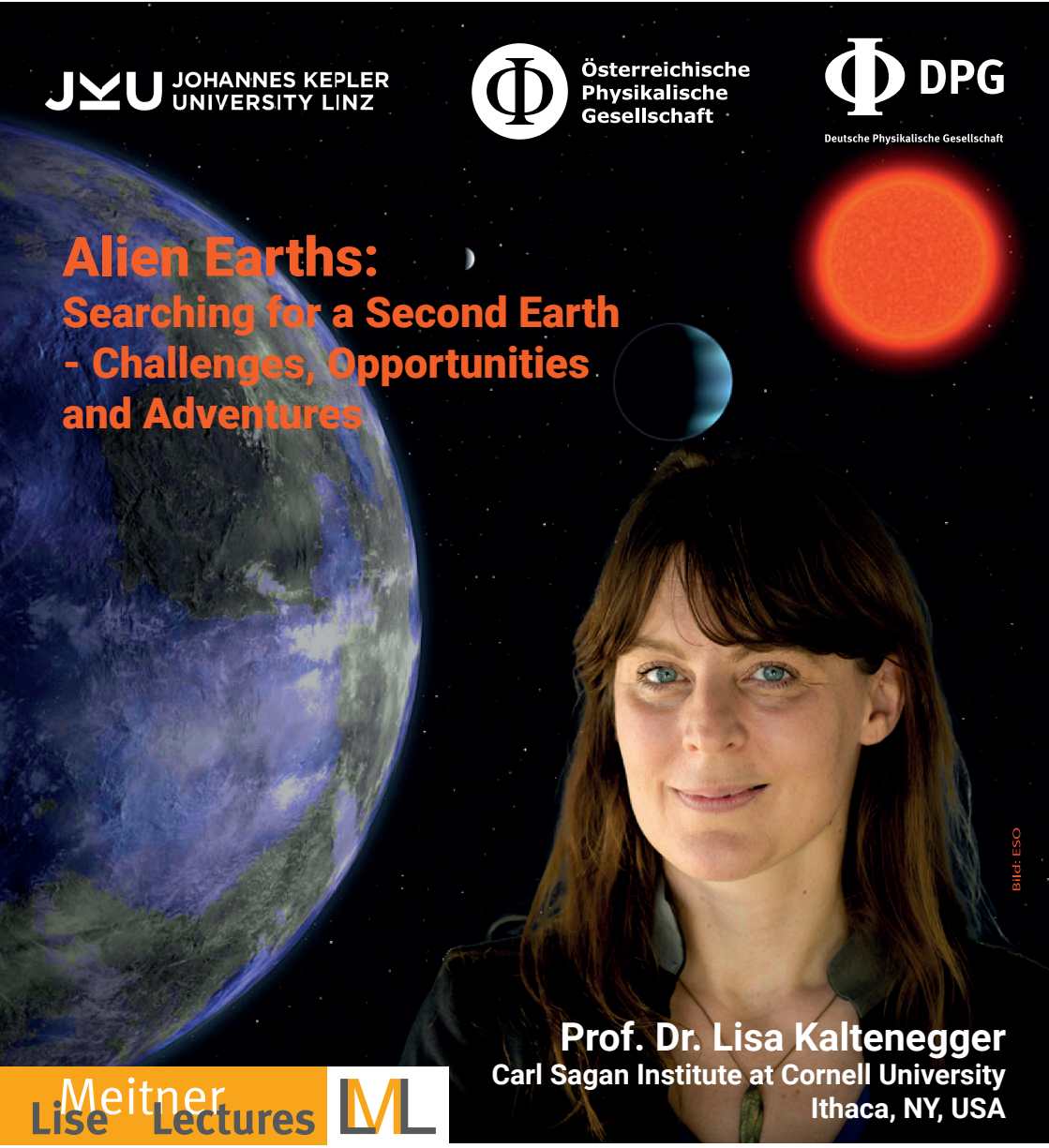

Bild: ESO

Prof. Dr. Lisa Kaltenegger
Carl Sagan Institute at Cornell University
Ithaca, NY, USA

Lise Meitner Lectures ML

Öffentlicher Abendvortrag
Johannes Kepler Universität Linz
Hörsaal 10
Altenberger Str. 69
4040 Linz

Montag, 23.09. 2024
18:30 - 20:00 Uhr

Eintritt frei.

www.lisakaltenegger.com
www.lise-meitner-lectures.de

Movie Screening

Tuesday, 24 September, 18:45, HS 10

Documentary movie in German language: **“Vom Sinn des Ganzen” (“On the meaning of everything”)** on the physicist **Hans-Peter Dürr** (1929-2014): directed by **Claus Biegert** (2020, 103 min.), who will be presenting his film and giving an introduction.

Claus Biegert follows the life of this unusual scientist in a dialogue with the American Sue Durham, who became Dürr's wife and taught him how to dance.

His doctoral supervisor was Edward Teller, the inventor of the hydrogen bomb. They argued for a lifetime. Werner Heisenberg appointed him as his successor at the Max Planck Institute. Hannah Arendt encouraged him to work as a border crosser. Josef Rotblat brought him to the table at his legendary Pugwash Conferences, which were honored with the Nobel Peace Prize. The physicist Hans-Peter Dürr was an agile thinker and an encourager. He doubted the existence of matter and focused on relationships and the in-between: Between particles, but also between trees, people and world powers. Knowledge that does not reach into the future is no knowledge at all. He cast his net around the globe and got involved. For this he received the Alternative Nobel Prize. The Potsdam Manifesto, which calls for peace with the earth and a strategic orientation towards the paradigm of the living, seems like his testament.

Prizes and Awards

The Austrian Physical Society is awarding several prizes to outstanding young academics, pupils and their theses.

1. **Fritz Kohlrausch Prize:** Awarded to young physicists for their experimental works
2. **Roman Ulrich Sexl Prize:** Awarded to excellent achievements in the field of teaching and didactical planning on any educational level
3. **ÖPG Dissertation Prizes:** for excellent PhD theses in Physics
4. **ÖPG Students Prizes**: for excellent Master and Diploma theses in the field of experimental or theoretical physics
5. **Prizes for pre-scientific physics theses**: for pupils graduating in the year 2023/24
6. **Max Auwärter Prize:** Awarded to an outstanding scientific thesis in the field of atomic physics, surface physics, interfacial chemistry, and anorganic and organic thin layers

Award Ceremony

The Award Ceremony will be taking place on Tuesday, 24 September, from 11:00 to 12:30 in HS 10

Awardee Talks

The awardee talks for Roman Ulrich Sexl Prize, Fritz Kohlrausch Prize and Max Auwärter Prize will be taking place on Wednesday, 25 September, from 11:00 to 12:30 in “OIC Stufenforum”.

Time schedule and program

Monday

11:00	Registration Raiffeisen Innovation Centre						11:00
11:15							11:15
11:30							11:30
11:45							11:45
12:00							12:00
12:15							12:15
12:30							12:30
12:45							12:45
13:00	Opening HS 10						13:00
13:15							13:15
13:30	Plenary Lecture 1 Michele Punturo HS 10						13:30
13:45							13:45
14:00							14:00
14:15	Break						14:15
14:30		Energy Day HS 17	COND 1 HS 09	Burgholzer	FAKT 1 HS 10	Reindl	14:30
14:45				Wagner		Simon	14:45
15:00				Hollweger		Murtagh	15:00
15:15				Pransu		Kraxberger	15:15
15:30				Aichner		Kilian	15:30
15:45				Keppert		Wagner	15:45
16:00	Break						16:00
16:15							16:15
16:30	ÖPG Executive Assembly MZ 003A	Energy Day HS 17	COND 2 HS 09	Worm	FAKT 2 HS 10	Wutte	16:30
16:45							16:45
17:00				Singh		Ecker	17:00
17:15				Adhikari		Mager	17:15
17:30				Krsnik		Mandl	17:30
17:45				Reddy		Koch	17:45
18:00	Break						18:00
18:15							18:15
18:30	Lise Meitner Lecture HS 10						18:30
18:45							18:45
19:00							19:00
19:15							19:15
19:30							19:30
19:45							19:45
20:00							20:00
20:15							20:15

Tuesday

09:00	Plenary Lecture 2 Brigitte Bach HS 10											09:00
09:15												09:15
09:30												09:30
09:45	Plenary Lecture 3 Fabio Crameri HS 10											09:45
10:00												10:00
10:15												10:15
10:30	Break											10:30
10:45												10:45
11:00	Award Ceremony HS 10											11:00
11:15												11:15
11:30												11:30
11:45												11:45
12:00												12:00
12:15												12:15
12:30	Lunch Break											12:30
12:45												12:45
13:00												13:00
13:15												13:15
13:30												13:30
13:45												13:45
14:00	(HS 8) YM 1	Siboni	Poster Session HS 17									14:00
14:15												14:15
14:30		Brückl										14:30
14:45												14:45
15:00		Albrecht										15:00
15:15												15:15
15:30	Break											15:30
15:45												15:45
16:00	(HS 8) YM 2	Pomper	(HS 9) ENS	Beisteiner	(HS 10) GEP	Sachslehner	(BA 9911) LHS	Schmid	(BA 9910) OGD 1	Resel		16:00
16:15				Preisinger		Folk		VWA		Schwarzl		16:15
16:30		Lightening Talks		Reichl		Draxler		Preisträger		Schiek		16:30
16:45				Reichl		Besser		*innen		Martinez		16:45
17:00		Quiz		Wesselak		Boudjada		[1]		Brozyniak		17:00
17:15				Chamasemani		Perez		[2]				17:15
17:30	Break											17:30
17:45												17:45
18:00	Plenary Lecture 4 Heinz Krenn HS 10											18:00
18:15												18:15
18:30												18:30
18:45	Movie Introduction & Screening HS 10											18:45
19:00												19:00
19:15												19:15
19:30												19:30
19:45												19:45
20:00												20:00
20:15												20:15

[1] – Vorst. IYPT Tournament; [2] – Vorst. Physikolympiade

Wednesday

08:30	Opening CECMD							08:30
08:45	HS 10							08:45
09:00	Plenary Lecture 5							09:00
09:15	Christoph Stampfer							09:15
09:30	HS 10							09:30
09:45	Plenary Lecture 6							09:45
10:00	Nicola Marzari							10:00
10:15	HS 10							10:15
10:30	Break							10:30
10:45								10:45
11:00	CECMD HF 9901 (special program)	Roman-Ulrich-Sexl Prize						11:00
11:15		OIC Stufenforum						11:15
11:30		Fritz-Kohlrausch Prize						11:30
11:45		OIC Stufenforum						11:45
12:00		Max-Auwärter Prize						12:00
12:15		OIC Stufenforum						12:15
12:30	Lunch Break							12:30
12:45								12:45
13:00								13:00
13:15								13:15
13:30								13:30
13:45								13:45
14:00	CECMD HF 9901 (special program)	AMP 1 HF 9904	Bruschi	FAKT 3 BA 9911	Ricaurte	OGD 2 BA 9910	Boné	14:00
14:15			Masiello		Jeitler			14:15
14:30			Wagner		Kneringer		Roy	14:30
14:45			Liang		Schotter		Blatnik	14:45
15:00			Ji		Stummer		Hütner	15:00
15:15			Kirova				Wagner	15:15
15:30	Break							15:30
15:45								15:45
16:00	CECMD HF 9901 (special program)	AMP 2 HF 9904	Chen	MBU BA 9911	16:00 Blank	OGD 3 BA 9910	Aschauer	16:00
16:15			Nguyen		16:20 Wilson			16:15
16:30			Gattinger		16:40 Buchberger		Klasen	16:30
16:45			Diez				Niggas	16:45
17:00			Krondorfer				Schwab	17:00
17:15							Khan	17:15
17:30								17:30
17:45								17:45
18:00								18:00
18:15								18:15
18:30	Break							18:30
18:45								18:45
19:00	Conference Dinner Promenadenhof, Promenade 39, 4040 Linz							19:00
19:15								19:15
19:30								19:30
19:45								19:45
20:00								20:00
20:15								20:15

Thursday

08:00	SFB Beyond C						08:30
08:30	Women's Breakfast @ Teichwerk						08:45
09:00	SFB BeyondC	Plenary Lecture 7 Marta Gibert HS 10					09:00
09:15							09:15
09:30	VOEST Alpine excursion						09:30
09:45		Plenary Lecture 8 Martina Erlemann HS 10					09:45
10:00							10:00
10:15							10:15
10:30		Break					10:30
10:45							10:45
11:00		OEPG Members Assembly HS 10					11:00
11:15							11:15
11:30							11:30
11:45							11:45
12:00	SFB BeyondC Business Meeting						12:00
12:15							12:15
12:30		Lunch Break					12:30
12:45							12:45
13:00	Lunch Break						13:00
13:15							13:15
13:30							13:30
13:45							13:45
14:00	SFB BeyondC König, Stefszky, Munoz-Gil	AKCP BA 9910	Götschel	COND 3 + NESY HS 9	David	PIN 1 HS 10	Schwarz	14:00
14:15			Blank					14:15
14:30			Sandner		Gvindzhiliia		Pachinger	14:30
14:45					Hameed			14:45
15:00					Lechner		Stadlober	15:00
15:15					Rauscher			15:15
15:30	Break							15:30
15:45								15:45
16:00	SFB BeyondC J. Kofler, G. Widmer			COND 4 HS 9	Kratzer	PIN 2 HS 10	Dinhobl	16:00
16:15					Mazza			16:15
16:30					Tang		Heidegger	16:30
16:45					Salchegger			16:45
17:00					Nasrallah		Schwabegger	17:00
17:15					Aichhorn			17:15
17:30	Break						Schwab	17:30
17:45								17:45
18:00	SFB BeyondC Reception @ Redoutensaal							18:00
18:15								18:15
18:30								18:30
18:45								18:45
19:00	Public Evening Lecture: Hans Briegel @Redoutensaal, Promenade 39, 4040 Linz							19:00
19:15								19:15
19:30								19:30
19:45								19:45
20:00								20:00
20:15								20:15

Energietag „Wasserstoff“ im Rahmen der ÖPG Jahrestagung 2024

Montag, 23.09.2024, 14:30-18:10

Johannes Kepler Universität Linz, Altenberger Straße 69,
4040 Linz, Österreich

HS 17 (Managementzentrum)

Begrüßung: Christian Teichert

Führung durch das Tagesprogramm: Robert Hauser, Christoph Reichl

14:40 Thomas Kienberger (Montanuniversität Leoben)	Österreichs Energiezukunft: Planung und Umsetzung mit besonderer Berücksichtigung des Themas Wasserstoff
15:25 Alexander Trattner (HyCentA Research GmbH, TU Graz)	Grüner Wasserstoff in Österreich: Erzeugung, Transport, Speicherung

16:10 Pause

16:30 Irmela Kofler (K1-MET GmbH)	Kohlenstoffarme Stahlerzeugung in der Zukunft
16:55 Margherita Matzer (WIVA P&G)	Hydrogen Valley – H2Real
17:20 Christopher Lamport (BMK, Allgemeine Klimapolitik)	Beitrag von erneuerbarem Wasserstoff zu Energiewende und langfristiger Klimaneutralität

17:45 Moderierte Diskussion (Moderator: Gero Vogl)

18:10 Ende des Energietags

18:30 Lise Meitner Lecture

Program Central European Condensed Matter Day

Time		Wednesday, 25 September 2024, HF 9901
8:30		Opening: Central European Condensed Matter Day
9:00		Plenary: **Christoph Stampfer** (RWTH Aachen), D
9:45		Plenary: **Nicola Marzari** (EPFL/PSI), CH
10:30		***Coffee break***
11:00		**Anna Coclite** (TU Graz/Univ. of Bari), A Thin films deposited from the vapor phase for smart sensors and beyond
11:30		**Levente Tapasztó** (EK-MFA Budapest), H Tuning the properties of 2D crystals by nanoscale strain and defect engineering
12:00		**Viera Skákalová** (Slovak Acad. Sci. Bratislava), SK Novel Two-Dimensional Materials Synthesized in Graphene Oxide Under Ambient Conditions: Atomic Structure and Properties
12:30		***Lunch***
13:30		**Andrej Zorko** (Jožef Stefan Inst. Ljubljana), SLO Quantum phases of rare-earth heptatantalates
14:00		**Ana Akrap** (Univ. of Zagreb), HR Magneto-optical insights into quantum materials
14:30		**Jakub Zelezny** (Czech Acad. Sci. Prague), CZ Non-Relativistic Spin Currents and Torques in Antiferromagnets
15:00		**Tomáš Bzdušek** (Univ. of Zurich), CH Unraveling the spectra and topological phases in hyperbolic lattices
15:30		***Grab a coffee***
15:45		Short presentations of infrastructures • CEITEC Nano, Brno, CZ • ELI ALPS laser center for attosecond experiments, Szeged, H

		• CALT - Centre for Advanced Laser Techniques Institute of Physics, Zagreb, HR • Centre of Low Temperature Physics, (IEP SAS and Šafárik University), Košice, SK • IonBeamCenter - Institute Ruđer Bošković, Zagreb, HR • Vienna Microkelvin Laboratory, TU Vienna, A & more
17:15		Panel discussion on the future of science education in the realm of online teaching and AI; exploring synergies through collaborative activities and student exchanges.
19:00		***Conference Dinner, Promenadenhof Linz***

CECMD program committee

Austria: Silke Buehler-Paschen (TU Vienna), Wolfgang Lang (U. Vienna)
Croatia: Ana Akrap (U. Zagreb), Denis Sunko, (U. Zagreb)
Czechia: Michal Urbánek (CEITEC Brno), Jan Kunes (U. Brno)
Hungary: Béla Pécz, (Hungarian Research Network Budapest), Szabolcs Csonka, (U. of Technology and Economics Budapest)
Slovakia: Milan Sýkora (U. Bratislava), Peter Samuely (Center for Low Temperature Physics Košice)
Slovenia: Dragan Mihailović (Jožef Stefan Inst. Ljubljana)
Switzerland: Johan Chang (U. Zurich), Henrik Rønnow (EPFL Lausanne)
Head of the Mid-EU Initiative: Neven Barišić (TU Vienna & U. Zagreb)
ÖPG organization committee:
Local organizers: Andreas Schell (JKU Linz), Gunther Springholz (JKU Linz)
ÖPG President: Christian Teichert
ÖPG Head of the Condensed Matter Section: Alberta Bonanni

AKCP Symposium: „Diversity, Equality & Inclusion"

Im Studium und im weiteren Verlauf einer Karriere in der Physik sollte Geschlecht keine Rolle spielen. Dennoch zeigen alltägliche Beobachtungen im Studium und am Arbeitsplatz, dass der Anteil der Frauen noch weit unter 30% liegt und Chancengleichheit nicht vollends erreicht wurde.

Im Rahmen dieses Symposiums des Arbeitskreises für Chancengleichheit in der Physik (AKCP) werden drei Impulsvorträge gehalten, die Diversität in der Physiklehre, Maßnahmen zur Verbesserung der Chancengleichheit, sowie Karriereeinblicke einer erfolgreichen Professorin adressieren. Die Zuhörenden werden anschließend eingeladen, im Symposium mitzudiskutieren und ihre Erfahrungen zu teilen.

Der AKCP der Österreichischen Physikalischen Gesellschaft (ÖPG) wurde 1992 gegründet, um die Anzahl der Frauen in der Physik zu erhöhen. Im September 2023 wurde der Arbeitskreis nach sieben Jahre Pause wieder reaktiviert.

Programm:

14:00-14:05	Begrüßung Andrea Navarro Quezada, Vorsitzende des AKCP der ÖPG
14:05-14:20	Helene Götschel, Europa Universität Flensburg, „Innovative, geschlechtergerechte Physiklehre an Hochschulen"
14:25-14:40	Kerstin Blank, Johannes Kepler Universität Linz, „Der unsichtbare Lebenslauf: Karriereeinblicke einer Professorin der ersten Generation"
14:45-15:00	Agnes Sandner, Arbeitskreis für Chancengleichheit der DPG „Der Arbeitskreis Chancengleichheit: Seine Bedeutung und die Projekte seit 25 Jahren"
15:00-15:30	Offene Diskussion; Moderation Hemma Bieser, Vorständin OurPower und Geschäftsführerin avantsmart

Das Symposium wird in deutscher Sprache abgehalten.

SFB BeyondC Autumn Workshop

September 26 2024

ÖPG Meeting JKU Campus Linz
BA 9911 (Bankengebäude, UG)

THURSDAY, 26.09.2024	
Time	**Program**
08:00 – 09:00	Women's Breakfast I Teichwerk (registration required)
09:00 – 09:30	Bus transfer
09:30 – 11:00	VOEST ALPINE I Plant tour (registration required)
11:00 – 11:30	Bus transfer
12:00 – 13:00	*SFB BeyondC* Business Meeting I Management-Zentrum
13:00 – 14:00	*SFB BeyondC* PI – Lunch
14:00 – 14:30	Robert König I TUM How to fault-tolerantly realize any quantum circuit with local operations
14:30 – 15:00	Michael Stefszky I UNI PADERBORN PaQS: The Paderborn Quantum Sampler
15:00 – 15:30	Gorka Munoz Gil I UIBK Generating quantum circuits with diffusion model
15:30 – 16:00	Coffee break
16:00 – 16:30	Johannes Kofler I JKU BruQner – The Sound of Entanglement
16:30 – 17:00	Gerhard Widmer I JKU AI, Machine Learning, and the Human Element in Music
18:00 – 19:00	SFB BeyondC Reception *
19.00	Public Evening Lecture Hans Briegel I UIBK *

* Redoutensäle / Promenade 39, 4020 Linz

Abstracts

Plenary lectures

#001	MON	PLENARY 1	13:30 – 14:15	HS 10

Einstein Telescope: the next generation European Gravitational Wave observatory

Michele Punturo[1]

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The current generation of gravitational wave (GW) detectors, Advanced Virgo and Advanced LIGO, have opened a new window on the Universe by detecting GW signals in the Hz-kHz frequency range. Monumental scientific goals have been achieved thanks to their observations. More recently, the Pulsar Timing Array experiments have just announced the detection of GWs in the nanohz frequency range.

A new generation of terrestrial and space-based interferometric GW observatories is being prepared to replace the current generation of GW detectors in the next decade. This will make it possible to search almost the entire Universe for GW signals. Einstein Telescope (ET) is leading the design, preparation and implementation of next-generation terrestrial GW observatory in Europe. ET aims to detect all stellar or intermediate-mass black hole mergers throughout the Universe, testing general relativity in the presence of a strong gravitational field. ET will detect a large fraction of the coalescences of binary neutron star systems in the Universe, shedding light on the equation of state that governs the physics of these compact bodies. ET will contribute to the understanding of dark matter and dark energy by looking at the gravitational side of this puzzle.

An overview of the scientific objectives, the observatory design, the required technologies and the project organization of Einstein Telescope is presented.

#002	TUE	PLENARY 2	09:00 – 09:45	HS 10

Wie exzellente Wissenschaft und Forschung wirksam werden

Brigitte Bach[1]

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Die „Triple Transition" – die gleichzeitig ablaufende ökologische und digitale Transformation, die menschengerecht sein soll – stellt große Herausforderungen, bietet aber auch große Chancen. Technologie bildet einen zentralen Baustein für Lösungen. Damit aus exzellenter und Forschung zukunftsfähige Innovationen werden, bedarf es einer ganzen Reihe von Schritten entlang der gesamten Innovationskette – von der wissenschaftlichen Idee über Prototypen bzw. Großdemonstratoren bis hin zur industriellen Entwicklung. Durch erfolgreiche Innovationen können wir die Herausforderungen aus der „Triple Transition" nutzen, um die Wettbewerbsfähigkeit der Wirtschaft und Industrie in Österreich zu steigern.

Brigitte Bach hat als Sprecherin der Geschäftsführung des AIT Austrian Institute of Technology die Verantwortung für die strategische Positionierung der Forschungseinrichtung sowie für Außenbeziehungen und Produktportfolio inne.

Die Physikerin Brigitte Bach war von 1999 bis 2018 maßgeblich an der Entwicklung und strategischen Positionierung der Energieforschung am AIT beteiligt, zuletzt als Leiterin des Center for Energy. Ab 2018 leitete sie bei Wien Energie die Bereiche Telekommunikation, Elektromobilität und neue Geschäftsfelder, danach war sie als Direktorin der Salzburg AG tätig.

How excellent science and research become effective

The "triple transition" – the simultaneous ecological and digital transformation that needs to be humane – poses major challenges, but also offers great opportunities. Technology is a central building block for solutions. Turning excellent research into sustainable innovations requires a whole series of steps along the entire innovation chain – from the scientific idea to prototypes and large-scale demonstrators through to industrial development. With the help of successful innovations, we can use the challenges from the "triple transition" to increase the competitiveness of the economy and industry in Austria.

As Spokesperson of the Management Board of the AIT, **Brigitte Bach** is responsible for the strategic positioning of the research institute as well as for external relations and the product portfolio.

Physicist Brigitte Bach played a key role in the development and strategic positioning of energy research at AIT from 1999 to 2018, most recently as Head of the Center for Energy. From 2018 on, she was Head of Telecommunications, Electromobility and New Business Areas at Wien Energie, after which she worked as Director of Salzburg AG.

#003	TUE	PLENARY 3	09:45 – 10:30	HS 10

The theory of ~~everything~~ accurate and accessible colour use

Fabio Crameri[1,2]

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In the vast landscape of scientific data, colour serves as a golden key to its comprehension. From the depths of the cosmos to the intricacies of elementary particles, the deliberate use of colour in scientific visualization enriches our understanding and enables us to appreciate the beauty and complexity of the natural world.

As of today, scientific visualization is rarely part of the obligatory curriculum of an upcoming physicist. In terms of colour use, the physics community therefore swings back and forth between self-educated science-proof application and peer-endorsed misuse. When misused, data visualization can exclude readers or misguide them. In the worst case, it does both.

From the properties of the light source to the ultimate recognition in the visual cortex, the study of human colour perception is extensive and has a long history. Creating accessible and accurate scientific visualization with colour has, in contrast, become easy. All necessary aspects are understood. All necessary tools exist.

Here, I will provide you with the basic understanding to use—and not misuse—colour for visualising everything from the *Standard Model of particle physics* to the *Island of Stability*. Pioneering science-proof colour palettes and gradients have left their island and appear now in great numbers conquering the continent. To avoid any form of colour confinement, I will also introduce you to the newest version of the Scientific colour maps and the different palette and gradient types available therein.

After just this one lecture (given you stay alert and I don't fall down the stage), you shall be equipped to navigate the most-basic use of colour in your daily routine. I also hope you will then become an advocate of the scientific use of colour yourself so that after having mastered our theory of everything, we as a community will not fail the one job left: to accurately show it to everybody else.

#004	TUE	PLENARY 4	18:00 – 18:45	HS 10

The pioneering development of physics until 1900 exemplified by the Historic Site Award "Physics Institute of the University of Graz"

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The EPS Historic Sites Award commemorates places in Europe important for the development and the history of physics. According to the European Physical Society (EPS), a necessary condition for nomination is evidence of pioneering achievements at places (laboratories, buildings) associated with research by one or more individuals, that made important contributions. This includes places where instruments and/or apparatus were designed making significant advances in physics. The Institute of Physics at the University of Graz, built from 1872-76 by August Töpler (1836-1912), is celebrating its 150th anniversary together with the 180th anniversary of the birth of Ludwig Boltzmann (1844-1906), the leading figure of the institute during his most fruitful scientific work from 1876-1890. As the most modern physics institute in Europe at the time, it attracted renowned scientists (Walther Nernst, Svante Arrhenius) and was even able to call two Nobel Prize winners (Viktor Franz Hess and Erwin Schrödinger) as full professors (who were then forced into exile by political circumstances in 1938). The building offered experimental possibilities, for example, to anticipate important findings about light and electromagnetism even before Maxwell's theory was established in continental Europe and before H. Hertz discovered electromagnetic waves (just as M. Faraday's experiments originally initialized Maxwell's theory of electromagnetism). Studies on electric transport in metals, galvano- and thermomagnetic effects (Albert von Ettingshausen) were probably only possible here, as a "iron-free" laboratory was created to suppress magnetic interference fields. Isolated vibration-free supporting pillars (throughout the building and in the astronomical tower) allowed high-precision optical and astronomical measurements. Incidentally, the building is experiencing a dèjá-vu with the new Graz Center of Physics, which will be completed in 2030 and unite the physics institutes of both Graz universities.

#005	WED	PLENARY 5	09:00 – 09:45	HS 10

Quantum Dots in Bilayer Graphene

Christoph Stampfer[1,2]

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Graphene and bilayer graphene (BLG) are promising materials for quantum technologies. Considerable effort has been devoted to the study of quantum dot (QD) devices based on these materials. The main challenge in using graphene for such applications is the lack of a band gap, which prevents electrostatic confinement of electrons. A common solution has been to physically etch graphene to create hard wall confinement, but this method is hampered by edge disorder, making it difficult to make clean quantum devices.

In contrast, BLG can circumvent the edge disorder problem due to its tunable bandgap (up to 120meV) when subjected to a perpendicular electric field, enabling electrostatic soft confinement. This talk will present recent progress in gate-controlled single and double quantum dot operations in electrostatically gapped BLGs. The devices demonstrate a high degree of control, enabling gate-defined electron-hole and electron-electron double quantum dot systems with single electron occupancy. Few-electron/hole states have been achieved in the single dot regime, with excited state energies extracted and analyzed under parallel and perpendicular magnetic fields.

Recent data on ultra-clean BLG quantum dots will be presented, highlighting the study of spin-valley coupling, electron-hole crossover and symmetry between electron and hole states. In addition, findings on BLG quantum dots focusing on spin and valley lifetimes will be discussed. This work lays the foundation for the development of spin and valley qubits in graphene.

#006	WED	PLENARY 6	09:45 – 10:30	HS 10

The shape of things to come: computational science driving scientific discovery and technological innovation

Nicola Marzari[1,2,3]

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Computational science has benefited for many decades from the algorithms and the hardware that have made it one of the greatest accelerators of research, with results and impact that run deep in science and technology The key challenges that it faces are those of predictive accuracy, with simulations able to capture the quantum nature of electrons and nuclei; of realistic complexity, aiming to describe ever more challenging systems; and of materials informatics, leveraging the disruptive capabilities of machine learning and artificial intelligence.

I'll highlight some of the key efforts we are targeting: addressing the electronic structure of compounds with strongly localized and correlated electrons, developing mesoscopic equations and formulations that bring atomistic and quantum precision to the macroscopic scale, and delivering automated capabilities that can be externalized and then orchestrated by human and not-so-human players.

Some example applications will cover materials for energy (Li-ion cathodes and solid-state conductors) and materials for information-and-communication technologies (2D and 1D materials, topological insulators, and superconductors).

#007	THU	PLENARY 7	09:00 – 09:45	HS 10

Magnetic double-perovskite oxide heterostructures

Marta Gibert[7]

J. Spring[1], N. Fedorova[2], A. B. Georgescu[3], G. De Luca[4], S. Jöhr[1], M. Rossell[5], C. Piamonteze[6], J. Íñiguez-González[2]

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Atomically-engineered heterostructures constitute excellent model systems for investigating fundamental structure-property relations in transition metal oxides and their evolution as the thickness of the constituent layers is reduced to only a few unit cells.

The double-perovskite RE_2NiMnO_6 (*RE*= rare earth) family is characterized as being insulating ferromagnets, an unusual combination of properties. Ferromagnetism arises through oxygen-mediated superexchange in the rock salt-ordered Ni/Mn sublattice. The Curie Temperature of La_2NiMnO_6 is T_c=280K, and for the other members of the family, T_c decreases linearly with the size of the ionic radius of the *RE*.

Here, we will show that epitaxial RE_2NiMnO_6 films (*RE*=La, Nd, Sm), grown by RHEED-enabled off-axis magnetron sputtering, display long-range Ni^{2+} and Mn^{4+} order and strain-independent bulk-like T_C at a thickness of 30 unit cells [1,2]. We find that the ferromagnetic behavior occurs down to ultra-low thicknesses of (at least) 3 unit cells (~1.2 nm). However, below 10 unit cells, the magnetic properties deteriorate due to an interfacial charge transfer caused by the polar discontinuity at the $RE_2NiMnO_6/SrTiO_3$ interface [2,3]. For the case of Nd_2NiMnO_6, a detailed x-ray magnetic circular dichroism (XMCD) study allows us to separate the magnetic components into a robust ferromagnetic Ni/Mn sublattice and a paramagnetic Nd sublattice.

We will also present our latest efforts in combining different RE_2NiMnO_6 double perovskites into potential multiferroic artificially-layered superlattices [4].

[1] G. De Luca et al., *APL Materials* 9, 081111 (2021).
[2] J. Spring et al., *Physical Review Materials* 7, 104407 (2023).
[3] G. De Luca et al., *Advanced Materials* 34, 2203071 (2022).
[4] H. J. Zhao et al., *Nature Communications* 5, 4021 (2014).

#008	THU	PLENARY 8	09:45 – 10:30	HS 10

Gender & Diversity in the Cultures of Physics

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In the last decades there has been a growing awareness that a scientist's gender can have an impact on a successful career in physics, even though it should have no influence. Moreover, also other categories of diversity and their impact on a career in science get more and more attention. The talk will present research on gender and diversity in physics with a particular focus on studies on the workplace cultures in physics and their impact on young scientists' sense of belonging to the physics community.

Abstracts

Awardee lectures

Max-Auwärter Prize				
#009	WED	AWARD 1	12:00 – 12:30	OIC Stufenforum

Investigating many-body phenomena through organic molecules and molecular nanostructures on surfaces

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The electronic structure of organic molecules, in particular polycyclic conjugated hydrocarbons, can be efficiently tailored through a rational design of molecular size, shape, and atomic structure of the edges, which can be used to generate unusual properties such as magnetism. As opposed to the localized nature of magnetic moments in transition metal atoms, unpaired electrons in organic molecules reside in delocalized molecular orbitals, which promotes efficient, tunable, and robust inter-molecular magnetic coupling.

Combining rational design principles with on-surface chemistry, I will show the generation of magnetism in polycyclic conjugated hydrocarbons, and its characterization by scanning probe techniques [1, 2]. The focus of this contribution will be on the bottom-up synthesis of all-organic $S = 1$ (S denotes the total spin quantum number) antiferromagnetic quantum spin chains on a Au(111) surface [3]. A systematic study of length-dependent magnetic excitations in both open-ended and cyclic spin chains reveals gapped spin excitations in the bulk, with the gap saturating for sufficiently long spin chains, and fractional $S = 1/2$ excitations at the chain termini, which manifest as Kondo resonances. It will be shown that these spectral features ratify Haldane's conjecture for integer-spin antiferromagnetic chains. Furthermore, the synthesis of an elusive organic molecule, namely, indeno[1,2-*a*]fluorene, will be demonstrated on ultra-thin insulating NaCl films on (111) coinage metal surfaces by means of scanning-probe-based atom manipulation [4]. The molecule exhibits ground-state bistability, wherein it can be stabilized either in a magnetic or a non-magnetic state, and can be switched between the two states by changing its adsorption site on the surface.

References:

[1] S. Mishra et al. Nature Nanotechnology 15, 22–28 (2020).

[2] S. Mishra et al. Nature Chemistry 13, 581–586 (2021).

[3] S. Mishra et al. Nature 598, 287–292 (2021).

[4] S. Mishra et al. Nature Chemistry 16, 755–761 (2024).

Fritz-Kohlrausch Prize				
#010	WED	AWARD 2	11:30 – 12:00	OIC Stufenforum

Unidirectional translation and cargo transport by a single molecule

Grant J. Simpson[1], M. Persson[2], and L. Grill[1]

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According to the principle of microscopic reversibility [1], in a thermally equilibrated system, the motion of individual molecules is random in nature. However, understanding how to control and direct motion of individual molecules is of importance and could lead to the production of novel materials or more efficient catalytic processes. Of great interest in this regard are molecular motors which display intrinsic directionality, that is, molecules which convert external energy into a predefined direction of motion. An example of such a system is the well-known Feringa motor [2]. However, such motors often show a reduction or loss of functionality when taken from their native solution phase and deposited onto a metallic surface.

In this talk a new concept in molecular motors will be demonstrated, which uses a small and simple chemical structure to achieve perfect unidirectionality when deposited onto a Cu(110) surface and investigated with a scanning tunneling microscope [3]. The motion is triggered by switching between two potential energy landscapes, thus avoiding microscopic reversibility, and leads to 100% unidirectionality in the molecule. Furthermore, this unidirectional motion can be harnessed to perform work by transporting small cargo molecules across the surface.

[1] R. C. Tolman, *Proc. Natl. Acad. Sci. USA*, **11**, 436–439 (1925)

[2] N. Koumura, et al. *Nature* **401**, 152–155 (1999)

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

Roman-Ulrich-Sexl Prize				
#011	WED	AWARD 3	11:00 – 11:30	OIC Stufenforum

Wie könnte ein moderner, motivierender Physikunterricht aussehen?

Erich Reichel[1]

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Der Physikunterricht hat sich in den letzten Jahrzehnten sehr verändert. Von einem lehrpersonzentrierten Unterricht, der sich oft nur an wenige Lernende richtete, hin zu einem stark die Forschungsmethoden nachzeichnenden, kooperativen Unterricht für alle. Dieser Paradigmenwechsel wurde in Österreich durch die ernste Wahrnehmung der Ergebnisse internationaler Untersuchungen (TIMSS, PISA) eingeleitet. Besonders durch das bundesweite Projekt IMST (Innovationen Machen Schulen Top) und die Einführung eines Kompetenzmodells für den naturwissenschaftlichen Unterricht wurden die Lehrpersonen der Naturwissenschaften motiviert, ihre best-practise-Modelle wissenschaftlich im Sinne der Aktionsforschung zu hinterfragen und untereinander auszutauschen. Der naturwissenschaftliche Unterricht wurde dadurch vom Schulsystem als unverzichtbarer Teil der (Allgemein)bildung wahrgenommen.

In den letzten Jahren wurden die Naturwissenschaften und die Technik weiter vernetzt, was durch den sogenannten MINT-Unterricht realisiert wurde. Eine wichtige Kombination, die junge Menschen dazu anleiten soll, Kompetenzen zu entwickeln, für das Leben in einer immer komplexer werdenden Welt mit all ihren Problemen. Eine immer stärker werdende Entwicklung der fachdidaktischen Forschung unterstützt dieses Vorhaben durch empirische Methoden. Dabei sollte aber nicht der Anschluss an die Physik als Fachwissenschaft verloren gehen.

Im Vortrag soll versucht werden, diesen modernen Physikunterricht an Hand von Beispielen, wie z.B. “Papier macht Schule”, “Physik mal anders” oder ein gut durchgeführtes Experiment zu illustrieren, und auf wesentliche Merkmale für einen gelingenden Physikunterricht hinzuwesen.

Abstracts

CECMD talks

#012	WED	CECMD	11:00 – 11:30	HF 9901

Thin films deposited from the vapor phase for smart sensors and beyond

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Fast response and large signal amplitude are fundamental requirements for good sensors. These properties can be achieved with stimuli-responsive materials: materials characterized by dynamic switching of their properties depending on external stimuli (e.g. light, pH, temperature, humidity). The deposition of such materials from the vapor phase allows to obtain low thicknesses with a sustainable-by-design process, since no solvents and extremely low quantities of chemicals are used. The thin film form allows obtaining fast response when such films are used as sensors. The process of initiated Chemical Vapor Deposition (iCVD), in addition, allows to obtain stimuli-responsive polymer thin films with high chemical specificity and this is important to obtain a large responsiveness amplitude.

A case of study will be presented in the field of artificial skins. Embedding sensors in smart architectures that record the response from the environment and transform it in a measurable signal is the objective of artificial skins. In this talk, a smart skin based on a single novel multi-stimuli responsive material, combining force, temperature and humidity sensing will be presented. The new sensor concept is realized by combining a hydrogel and a piezoelectric material in an array of core-shell structures. This architecture is achieved thanks to the use of vapor-based technologies for material processing, i.e. chemical vapor deposition, atomic layer deposition. We demonstrate that the skin can detect the stimuli with lateral resolution below the one of human skin. Possible applications stem from robotics to smart prostheses. Smart skins could monitor human breathing, pulse and temperature or detect dehydration.

#013	WED	CECMD	11:30 – 12:00	HF 9901

Tuning the properties of 2D crystals by nanoscale strain and defect engineering

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2D materials possess many intriguing properties, but one of their most attractive qualities is their fully accessible atomic structure that can be tuned much more efficiently, compared to bulk materials, in order to engineer their properties. Strain engineering the atomic structure of graphene, 2D MoS_2 and $ZrTe_5$ crystals with nanometre precision, enables the edge-free confinement of electronic states and surface plasmons in graphene, induces a direct to indirect bandgap transition in 2D MoS_2, and enables a transition from a weak to a strong topological insulator state in the band structure of $ZrTe_5$. Defects also play an important role in defining the properties of 2D materials. They can be employed to impart novel, often useful properties to various 2D crystals. Sulphur atom vacancies and substitutional oxygen atoms activate the basal plane of 2DMoS_2 crystals for various catalytic reactions, while Mo atom vacancies in 2D $MoSe_2$ display electrically tunable magnetic moments. Furthermore, defects of otherwise inert 2D crystals can also be exploited as anchor sites for their chemical functionalization with various molecules or even nanoparticles, giving rise to hybrid materials with novel properties.

#014	WED	CECMD	12:00 – 12:30	HF 9901

Novel Two-Dimensional Materials Synthesized in Graphene Oxide Under Ambient Conditions: Atomic Structure and Properties

V. Skákalová[1,2], P. Kotrusz[1,2], K. Mustonen[3], T.A; Bui[3], M. Precner[1], P. Hutár[1], M. Hulman[1,2], M. Orendač[4] and M. Gmitra[4]

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[2]*Danubia NanoTech, s.r.o., Slovakia*
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We have recently developed a simple chemical method SinGO (Synthesis in Graphene Oxide) that, under ambient conditions, can provide novel two-dimensional (2D) materials in a macroscopic scale [1]. The SinGO method opens an avenue to a new class of 2D magnetic and non-magnetic metal-iodides (2D-MI) encapsulated between graphene monolayers. Such vdW stacks would serve as a novel platform for nanotechnological devices in which 2D magnets hold spin whereas graphene as a conducting channel of Dirac electrons can guide the encoded relevant information. Noting that graphene spintronics has been aiming to exploit the extraordinary Dirac electronic properties but weak spin orbit-coupling limits its applicability for generating spin currents or spin torques. The proximity-induced spin-orbit coupling and exchange interactions in graphene-encapsulated 2D-MI magnets heterostructure might enable spin transport with unexplored yet physical mechanisms.

Here we will present the wide range characterization of 2D (magnetic and non-magnetic) metal-iodides encapsulated in graphene including their atomic structures (STEM), magnetization and electrical transport properties for possible applications.

References

[1] K. Mustonen et al., Toward Exotic Layered Materials: 2D Cuprous Iodide, *Advanced Materials* 34, 2106922 (2022).

#015	WED	CECMD	13:30 – 14:00	HF 9901

Quantum phases of rare-earth heptatantalates

A. Zorko[1,2]

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Antiferromagnetic materials generally undergo long-range magnetic ordering at temperatures lower than those set by their dominant exchange interactions. However, in specific instances, quantum fluctuations give rise to states that markedly deviate from classical magnetic orders. Notably, triangular antiferromagnets, which conventionally undergo classical ordering in the case of the Heisenberg isotropic nearest-neighbor exchange model, can manifest more intricate quantum states when deviations from this model occur. One such state is the spin supersolid, characterized by the coexistence of solid and superfluid properties. Another prominent example is the quantum spin liquid (QSL), which lacks long-range order even at zero temperature but maintains a high degree of quantum entanglement.

Our recent investigation has identified a QSL ground state in the novel triangular-lattice antiferromagnet neodymium heptatantalate, $NdTa_7O_{19}$ [1]. Comprehensive experiments revealed absence of magnetic ordering at temperatures significantly lower than the exchange interaction scale characteristic of this compound. Additionally, substantial Ising-like spin correlations between nearest neighbors on the triangular lattice and persistent spin dynamics were observed in the effective spin-1/2 ground-state Kramers doublet. This behavior was attributed to pronounced magnetic anisotropy of the Ising type.

Due to the typically large and highly specific magnetic anisotropy of rare earth (RE) ions, the extensive family of RE heptatantalates, $RETa_7O_{19}$ [2], offers a promising platform for exploring the complex quantum phases of triangular antiferromagnets. Recent experimental investigations have identified the erbium-based compound $ErTa_7O_{19}$ as a particularly promising member of this family. Moreover, recent progress in theoretical understanding of the intriguing phases of the triangular antiferromagnets highlights the critical role of the strength of the Ising anisotropy [3].

[1] T. Arh *et al*., *Nat. Mater*. **21**, 416 (2022).

[2] L. Wang *et al*., *J. Alloys Compd.* **937**, 168390 (2023).

[3] M. Ulaga *et al.*, *Phys. Rev. B* **109**, 035110 (2024).

#016	WED	CECMD	14:00 – 14:30	HF 9901

Magneto-optical insights into quantum materials

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I will give a broad overview of our recent progress on Landau level spectroscopy of Dirac and Weyl semimetals. With infrared light, one can excite carriers from one Landau level into another, causing inter-Landau level transitions. This technicque, known as Landau level spectroscopy, has been widely employed since the early 1950s as an extremely sensitive probe of semimetal and semiconductor band structures.

Through recent advances, one can resolve intricate complexities of topological materials' bands, all while discovering new physics. I will present highly detailed inter-Landau level transition maps in extreme magnetic fields, focusing on select topological materials: Dirac semimetals [1,2], a weak topological insulator $ZrTe_5$ [3,4], and a Weyl semimetal TaAs [5]. I will discuss how we can apply magneto-optical techniques to confirm or eliminate possible magnetic topological semiconductors [6].

[1] D. Santos-Cottin, M. Casula, L. de' Medici, F. Le Mardelé, J. Wyzula, M. Orlita, Y. Klein, A. Gauzzi, A. Akrap, R. P. S. M Lobo, "Universal optical features of Dirac cone networks: The case of BaNiS2 and their impact on the low-energy electronic structure", Phys. Rev. B 104, L201115 (2021).

[2] F. Le Mardelé, J. Wyzula, I. Mohelsky, S. Nasrallah, M. Loh, S. Ben David, O. Toledano, D. Tolj, M. Novak, G. Eguchi, S. Paschen, N. Barisic, J. Chen, A. Kimura, M. Orlita, Z. Rukelj, Ana Akrap, and D. Santos-Cottin "Evidence of 3D Dirac conical bands in TlBiSSe by optical and magneto-optical spectroscopy", Phys. Rev. B 107, L241101 (2023).

[3] E. Martino, I. Crassee, G. Eguchi, D. Santos-Cottin, R.D. Zhong, G.D. Gu, H. Berger, Z. Rukelj, M. Orlita, C. C. Homes, Ana Akrap, "Two-dimensional conical dispersion in ZrTe5 evidenced by optical spectroscopy", Physical Review Letters 122, 217402 (2019).

[4] I. Mohelsky, J. Wyzula, B. A. Piot, G. D. Gu, Q. Li, A. Akrap, and M. Orlita, "Temperature dependence of the energy band gap in ZrTe5: Implications for the topological phase", Phys. Rev. B 107, L041202 (2023).

[5] David Santos-Cottin, Jan Wyzula, Florian Le Mardelé, Iris Crassee, Edoardo Martino, Gaku Eguchi, Zoran Rukelj, Mario Novak, Milan Orlita, Ana Akrap, "Addressing shape and extent of Weyl cones in TaAs by Landau level spectroscopy", Phys. Rev. B 105, L081114 (2022).

[6] D. Santos-Cottin, I. Mohelský, J. Wyzula, F. Le Mardelé, I. Kapon, S. Nasrallah, N. Barisic, I. Zivkovic, J. R. Soh, F. Guo, M. Puppin, J. H. Dil, B. Gudac, Z. Rukelj, M. Novak, A. B. Kuzmenko, C. C. Homes, Tomasz Dietl, M. Orlita, and Ana Akrap, "EuCd2As2: a magnetic semiconductor", Phys. Rev. Lett. 131, 186704 (2023)

#017	WED	CECMD	14:30 – 15:00	HF 9901

Non-Relativistic Spin Currents and Torques in Antiferromagnets

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Contrary to the early understanding of antiferromagnets as limited compared to ferromagnets, a rich landscape of phenomena in antiferromagnets has been demonstrated that could be utilized for various spintronics functionalities. Here, we discuss recent advances in understanding of how electrical current can induce spin currents or spin torques in antiferromagnetic systems, focusing primarily on non-collinear antiferromagnets and on phenomena that originate from the non-collinear order without requiring the relativistic spin-orbit coupling. We show that antiferromagnets can host spin-polarized currents and that these can be utilized for magnetic junctions, that antiferromagnets can be used for spin-charge conversion, potentially even without any spin loss, and that a non-relativistic current-induced torque analogous to the spin-orbit torque can exist in antiferromagnets.

#018	WED	CECMD	15:00 – 15:30	HF 9901

Unraveling the spectra and topological phases in hyperbolic lattices

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Hyperbolic lattices are a new kind of synthetic matter with emergent negative curvature, realized over the past five years in various experiments, including coupled microwave resonators, electric-circuit networks, and silicon photonics. In the presence of open boundaries, hyperbolic lattices exhibit a large boundary-to-bulk ratio that remains finite in the thermodynamic limit, making them an attractive platform for realizing and enhancing topological edge modes. However, theoretical characterization of such systems is hindered by elusive non-Abelian Bloch states, which transform in higher-dimensional representations of a non-commutative translation group and that dominate the bulk energy spectrum.

In this talk, I will first clarify the concept of negative curvature and review the current understanding of space group symmetry and band theory in hyperbolic lattices [1]. Then, I will present our recent findings, focusing in particular on the newly formulated "supercell method" [2]. This method enables efficient computation of bulk spectra for a broad range of hyperbolic tight-binding models, accurately accounting for the non-Abelian Bloch states. Finally, I will briefly showcase applications of the supercell method to several hyperbolic lattice models, including a topological semimetal and a spin liquid characterized by non-vanishing first and second Chern numbers [3, 4].

[1] I. Boettcher, A. V. Gorshkov, A. J. Kollár, J. Maciejko, S. Rayan, and R. Thomale, *Crystallography of hyperbolic lattices*, Phys. Rev. B **105**, 125118 (2022).

[2] P. M. Lenggenhager, J. Maciejko, and T. Bzdušek, *Non-Abelian Hyperbolic Band Theory from Supercells*, Phys. Rev. Lett. **131**, 226401 (2023).

[3] T. Tummuru, A. Chen, P. M. Lenggenhager, T. Neupert, J. Maciejko, and T. Bzdušek, *Hyperbolic Non-Abelian Semimetal*, Phys. Rev. Lett. **132**, 206601 (2024).

[4] P. M. Lenggenhager, S. Dey, T. Bzdušek, and J. Maciejko, *Hyperbolic Spin Liquid* (in preparation, 2024)

Abstracts

Energy Day

#ED1	MON	Energy Day	14:40 – 15:25	HS 17

Österreichs Energiezukunft: Planung und Umsetzung mit besonderer Berücksichtigung des Themas Wasserstoff

Thomas Kienberger[1]

[1]*Montanuniversität Leoben*

Österreich hat sich zum Ziel gesetzt, den Strombedarf bis 2030 (bilanziell) zu einhundert Prozent aus erneuerbarer Energie zu decken. Die EU will als erster großer Wirtschaftsraum bis 2050 Klimaneutralität erreichen. Diese Ziele innerhalb des ambitionierten Zeitrahmens zu erreichen, bedingt eine konsistente und integrierte, systemische Planung. Die Arbeiten aus dem ÖNIP – dem österreichischen, integrierten Netzinfrastrukturplan – der in enger Abstimmung zwischen dem BMK und der Wissenschaft entstanden ist - liefert hierzu bereits eine gute, und in der EU bisher einzigartige Basis. Im Zentrum steht dabei eine integrierte Planung, die die hochrangigen Netzinfrastrukturen insbesondere für Strom und gasförmige Energieträger im Zentrum hat und aufzeigt, wie diese Richtung der geforderten Systemintegration weiterentwickelt werden müssen. Obwohl das Stromsystem aufgrund des sehr raschen Ausbaus dezentraler Erneuerbarer als Taktgeber der Veränderung oftmals im Zentrum der Wahrnehmung steht, ist eine Weiterentwicklung der Gas-Infrastruktur genauso wichtig. Diesem Aspekt widmet sich der gegenständliche Vortrag und fokussiert dabei auf das Thema Wasserstoff. Es gilt trotz großer Unsicherheiten, robuste Planungsgrundlagen in Bezug auf den Hochlauf der Bedarfsmengen, der inländisch erzeugte Mengen, der benötigten Infrastrukturen sowie der Kostensituation zu schaffen. Allen (teils unverständlichen) Hypes zum Trotz, ist doch eine sichere Versorgung mit Wasserstoff zentral, um einerseits die Produktion der energieintensiven Eisen- und Stahl- bzw. Chemieindustrie auch zukünftig sicherzustellen sowie anderseits den Ausgleich der volatilen Erneuerbaren im Stromsektor zu gewährleisten.

#ED2	MON	Energy Day	15:25 – 16:10	HS 17

Grüner Wasserstoff in Österreich: Erzeugung, Transport, Speicherung

Alexander Trattner[1]

[1]HyCentA Research GmbH, Technische Universität Graz, Institut für Thermodynamik und nachhaltige Antriebssysteme

Dieser Vortrag skizziert die Forschung, den technologischen Fortschritt und die industriellen Anwendungen von grünem Wasserstoff, der eine zentrale Rolle beim Übergang zu nachhaltigen Energiesystemen spielt. HyCentA, Österreichs führendes Wasserstoff-Forschungszentrum, verfügt über mehr als 19 Jahre Erfahrung und eine hochmoderne Infrastruktur, die eine breite Palette von Wasserstofftechnologien unterstützt. Der Status quo und die Entwicklungspotenziale entlang der gesamten Wertschöpfungskette des grünen Wasserstoffs werden vorgestellt. Dies umfasst Elektrolyse und Power-to-X, Grüne Energie und Industrie, Speicherung, Verteilung und Sicherheit von Wasserstoff, Grüne Mobilität sowie Kreislaufwirtschaft und die Verbesserung der Wasserstoffsysteme durch fortschrittliche Technologien

#ED3	MON	Energy Day	16:30 – 16:55	HS 17

Kohlenstoffarme Stahlerzeugung der Zukunft

Irmela Kofler[1]

[1]K1-MET GmbH

Im Pariser Klimaabkommen von 2015 einigte man sich auf eine maximale globale Temperaturerhöhung von 1,5°C bis zum Jahr 2100. Später wurde dies relativiert durch die Vorgabe einer CO2-Neutralität bis 2050 gemäß dem EU Green Deal und dem „Fit-for 55“ Paket (keine netto CO2-Emission bis 2050). Die österreichische Regierung setzt sich ambitionierte Ziele (100% elektrische Energie aus erneuerbaren Quellen bis 2030, Klimaneutralität bis 2040). Der Vortrag zeigt Dekarbonisierungspfade, welche von der Stahlindustrie eingeschlagen werden, um die Energiewende und Transformation zu klimaneutralen und effizienten Prozessen voranzutreiben. Dazu zählt auch Sektorkopplung, d.h., CO2 aus metallurgischen Prozessen als Rohstoff für effiziente industrielle Symbiosen zwischen energie- und ressourcenintensiven Sektoren. Hier spielen erneuerbare elektrische Energie und in weiterer Folge hergestellter „grüner“ Wasserstoff wesentliche Rollen. Im Beitrag werden laufende Forschungsprojekte als use cases herangezogen, um zu zeigen, wie die Herausforderung einer effizienten saisonalen Speicherung erneuerbarer elektrischer Energie durch Wasserstoff gemeistert werden kann und welchen Beitrag die Stahlindustrie dabei leistet.

#ED4	MON	Energy Day	16:55 – 17:20	HS 17

Hydrogen Valley – H2Real

Margherita Matzer[1]

[1]*WIVA P&G*

Damit Wasserstoff seine tragende Rolle in einem erneuerbaren Energiesystem übernehmen kann, muss eine nachhaltige Wasserstoffwirtschaft aufgebaut werden. Dafür benötigt es mehr als ein paar alleinstehende Vorzeigeprojekte, es benötigt ein Zusammenspiel aller Akteure entlang der gesamten Wasserstoffwertschöpfungskette. Um dieses Zusammenspiel bewerkstelligen zu können, ist das Konzept der Hydrogen Valleys ins Leben gerufen worden. Ein Hydrogen Valley ist ein geografisches Gebiet in dem grüner Wasserstoff produziert und lokal in verschiedenen Anwendungsbereichen genutzt wird. Durch Einbeziehen der lokalen Betriebe und Aufklärung der Bevölkerung wird ein stabiles System aufgebaut, dass in einem weiteren Schritt über Wasserstoffkorridore mit anderen Hydrogen Valleys verbunden werden kann. In der Ostregion von Österreich haben sich 17 Partner zusammengetan, um den Grundstein eines Hydrogen Valleys zu legen. Im Projekt H2Real (Hydrogen Region East Austria goes Live) wird ein integriertes H2-Netzwerk als Schlüssel für die Wasserstofftechnologie und -Anwendungen aufgebaut. Dabei werden sowohl bestehende als auch neue Technologien entlang der gesamten Wasserstoffwertschöpfungskette integriert und eine innovative und ganzheitliche Lösung entwickelt. Zusätzlich werden Stakeholder Workshops über Ländergrenzen hinaus organisiert, um alle Akteure der Region für ein Hydrogen Valley mit on-Board zu bekommen. Der gesamte Prozess von der Idee zum Hydrogen Valley wird in dem Vortrag erläutert und durch Beispiele an einzelnen Teilprojekten anschaulich dargestellt.

#ED5	MON	Energy Day	17:20 – 17:45	HS 17

Beitrag von erneuerbarem Wasserstoff zu Energiewende und langfristiger Klimaneutralität

Christopher Lamport[1]

[1]BMK, Allgemeine Klimapolitik

Die Europäische Union hat sich im „EU Climate Law“ das verbindliche Ziel gesetzt, bis 2050 die Klimaneutralität zu erreichen. Die Geschwindigkeiten der Mitgliedstaaten auf dem Weg dorthin werden unterschiedlich sein. Das Regierungsprogramm 2020-2024 enthält das politische Ziel der Klimaneutralität für Österreich bis 2040. Ein Erreichen dieses ambitionierten Ziels setzt ein rasches Umsetzen verschiedener Politiken und Technologien voraus. Erneuerbarer Wasserstoff ist dabei ein wichtiger Baustein, aber längst nicht der einzige. Wasserstoff kann vor allem in schwer zu dekarbonisierenden Bereichen eine wichtige Rolle spielen, in denen Elektrifizierung aus technischen oder wirtschaftlichen Gründen nicht immer möglich ist. Hierzu zählen neben der chemischen Industrie und Raffinerie energieintensive Industrieprozesse wie die Stahlerzeugung und Hochtemperatur-Prozesswärme, sowie der Einsatz in bestimmten, schwer elektrifizierbaren Bereichen in der Mobilität, wie z. B. Langstrecken Luft- und der maritime Schiffsverkehr und Teile des Schwerverkehrs. Die rechtlichen und wirtschaftlichen Rahmenbedingungen für den Aufbau eines Wasserstoffsystems werden sukzessive geschaffen. Neben dem Aufbau von Elektrolysekapazitäten für die Erzeugung von erneuerbarem Wasserstoff im Inland wird auch einer grenzüberschreitenden Transportinfrastruktur eine essenzielle Rolle zukommen.

Abstracts

Technical meetings of divisions

#019	MON	COND 1	14:30 – 14:45	HS 9

Controlled oxidation of exfoliated MoS_2

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Two dimensional (2D) semiconductors like molybdenum disulphide (MoS_2) belonging to the family of transition metal dichalcogenides, show electronic and optical properties relevant for applications ranging from nanoelectronics to sensorics and photonics [1]. Thermal annealing is generally involved in the fabrication of such devices in order to remove contaminants or to tune the electronic properties. In two-terminal memristive devices fabricated from oxidized MoS_2 the migration of oxygen (O) ions plays a major role in the switching mechanism [2], whose performance is crucial for applications in the next generation of memories and elements for neuromorphic computing.

A fundamental study of second harmonic generation and Raman spectroscopy on exfoliated MoS_2 flakes, with a thickness ranging from one up to eight monolayers as a function of the oxidation level, has been carried out. The controlled oxidation of the MoS_2 flakes on SiO_2 and on glass substrates is performed in a rapid thermal annealer, by varying the process time at a fixed temperature of 300°C. Samples non-treated and annealed in nitrogen atmosphere are considered, in order to elucidate the role of O in the process. This provides quantitative information on the oxidation mechanism and insights into how the oxidation of O base planes in the MoS_2 layers takes place, depending on the specific annealing parameters, resulting in either an alloy $MoS_{2-x}O_x$, or in fully oxidized MoO_x layers.

The results yield insights into the oxidation mechanism of atomically thin MoS_2 and confirm the relevance of the substrate and the number of monolayers for the reliability and performance of MoS_2-based devices. The findings contribute to the controllability of the fundamental physical and chemical properties of oxidized MoS_2.

[1] S. Xu, *et al*., in 2D Materials, 3(2), 021007 (2016).
[2] M. Wang, *et al.* Nat. Electron. 1.2 (2018): 130-136.

#020	MON	FAKT 1	14:30 – 14:45	HS 10

COSINUS: a new dark matter search experiment at the LNGS underground laboratory

F. Reindl[1,2] on behalf of the COSINUS collaboration

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Dark matter is one of the big unresolved problems of modern (particle) physics. Precision astronomy and cosmology prove that dark matter exists and that it is five times more abundant in the universe than ordinary matter, but the nature of dark matter has not been deciphered so far.

Direct detection experiments aim to solve this riddle by observing dark matter particles interacting in earth-bound detectors; the results, however, contradict: the DAMA/LIBRA experiment observes an annual modulation signal at high confidence that is perfectly compatible in terms of period and phase with the expectation for a galactic halo of dark matter particles interacting in their NaI target crystals. However, in the so-called standard scenario on dark matter halo and dark matter interaction properties, the DAMA/LIBRA signal contradicts the null results of numerous other experiments.

The new experiment COSINUS aims for a model-independent cross-check of the DAMA/LIBRA signal. Such a cross-check has been absent for now and necessarily requires using the same target material (NaI). COSINUS is the only NaI-based experiment operating NaI as a cryogenic detector, which yields several distinctive advantages: discrimination between electronic interactions and nuclear recoils off sodium and iodine on an event-by-event basis, a lower nuclear recoil energy threshold, and a better energy resolution. We finished the construction of the COSINUS experiment at LNGS in 2023; the cryostat is already running at base temperature. In this contribution, we will report on the prototype demonstrator measurement and give an outlook on the last steps towards the start of the data taking.

#021	MON	COND 1	14:45 – 15:00	HS 9

Structural and magnetic properties of exfoliated van der Waals layered $CrTe_2$ flakes

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Intrinsic magnetism in crystalline van der Waals (vdW) layered materials have emerged as the workbench for the exploration of collective magnetic phenomena down to 2-dimensional limits and are considered to be the building blocks for spintronics, memory devices and quantum magnonics. Within the family of vdW ferromagnets, the family of Cr-Te compounds are of particular interest, due to the diverse range of chemical stoichiometries attributed to the mechanism of Cr self-intercalation during the crystal growth, both in bulk and in thin films and ferromagnetic Curie temperature T_c which were reported to be in the range of 100 K – 320 K. These binary Cr_xTe_y compounds consist of $CrTe_2$ layers in which Cr atoms have an octahedral local environment with covalent Cr bridges between the layers. The magnetic properties of the Cr_xTe_y compounds are therefore dictated by the density of the Cr bridges. The compound expected to have the simplest coordination, the highest lamellar structure and air stability is 1*T*-$CrTe_2$.

Here, the structural, chemical and magnetic properties of mechanically exfoliated flakes of 1*T*-$CrTe_2$ are studied by employing atomic force microscopy (AFM), Raman spectroscopy, x-ray photoelectron spectroscopy (XPS) and low-*T*/high-$\mu_0 H$ magnetotransport measurements. The 1*T*-$CrTe_2$ flakes of thickness ~40 nm are mechanically exfoliated from a commercially obtained bulk crystal and transferred onto prepatterned SiO_2 (90 nm)/Si substrates using deterministic dry transfer technique. By combining Raman spectra and XPS of the flakes, a stoichiometry of Cr:Te = 0.6:1 corresponding to $Cr_{4.8}Te_8$ instead of the nominal 0.5:1 is found. The deviation of Cr:Te ratio from the nominal 1*T*-$CrTe_2$ is attributed to the presence of Te vacancies in the bulk crystal. The low-*T*/high-$\mu_0 H$ magnetotransport measurements show a metallic behavior in the flakes with a ferromagnetic Curie temperature T_c ~130 K and hysteretic magnetoresistance. The presence of ferromagnetic interaction in addition to its air stability make 1*T*-$CrTe_2$ a system of choice for vdW spin device applications.

#022	MON	FAKT 1	14:45 – 15:00	HS 10

Tests of CPT and Lorentz invariance by hydrogen and deuterium hyperfine measurements

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Hyperfine structure measurements on antihydrogen can provide sensitive tests of CPT invariance. The ASACUSA collaboration proposed such experiments on a beam of antihydrogen at the antiproton decelerator of CERN. We benchmark spectroscopy methods and equipment in supporting matter experiments. Beyond the relevance for antihydrogen these measurements can put new or improved constraints on specific coefficients of the so-called standard model extension (SME). Thereby CPT and Lorentz invariance is tested even without comparison to antihydrogen.

We have constructed an atomic beam setup for Rabi spectroscopy and performed such measurements for hydrogen at CERN and for deuterium at the Laboratoire Aimé Cotton, Université Paris-Saclay. We obtain constraints, e.g., on the SME non-relativistic (NR) anisotropic proton coefficients $\mathcal{T}_{p010}^{NR,Sun}$ by hydrogen and at higher fermion momentum power (k=2,4) on $\mathcal{T}_{pk11}^{NR,Sun}$ by deuterium, both on the order of 10^{-20} GeV. Determinations of the zero-field hyperfine splitting give agreement with literature (i.e. maser measurements) and the achieved levels of precision around 1 Hz for both atoms present the best values obtained by in-beam spectroscopy in each case. Finally, the relevance of the hydrogen measurements for antihydrogen spectroscopy will be discussed.

#023	MON	COND 1	15:00 – 15:15	HS 9

Superconducting proximity effect in $NbSe_2/ZrTe_5$ van der Waals heterostructures

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The technological prospect of Majorana zero modes and their role in fault tolerant quantum computing have been the main motivation behind the exploration of topological superconductivity. The superconducting proximity effect (SPE) in a topological quantum material/superconductor (TQM/SC) heterostructure is expected to induce superconducting energy gaps in the topological surface states of the TQM. Among the rich class of topological classes, the topological semimetals, namely Dirac semimetals, Weyl semimetals and nodal line semimetals (NLSM) are characterized by discreet gapless nodes. Fermi arcs and anomalous electromagnetic responses, such as the chiral magnetoelectric effect, are considered to be potential topological system to realize Majorana modes.

In this work, the SPE in the layered van der Waals (vdW) heterostructure $NbSe_2/ZrTe_5$, where $NbSe_2$ is a *s*-wave superconductor and $ZrTe_5$ a NLSM, is studied by employing low-T/high-$\mu_0 H$ magnetotransport. The structural properties and air stability of the mechanically exfoliated flakes of $NbSe_2$ and $ZrTe_5$ are investigated using Raman spectroscopy and x-ray photoelectron spectroscopy. The vdW heterostructure is fabricated using deterministic dry transfer onto SiO_2/Si substrate prepatterned with Pt electrodes for electrical contacts. The superconducting transition temperature T_c of the 20 nm $NbSe_2$ flake is found to be 6.8 K. The bulk superconducting energy gap Δ_b of the $NbSe_2$ layer and the surface superconducting energy gap Δ_s of the $ZrTe_5$ layer due to the SPE is investigated using differential conductance technique as a function of T and $\mu_0 H$ in a non-local geometry. The mechanism behind the proximity induced superconductivity in the NLSM and its correlation to the topological states along the nodal lines of $ZrTe_5$ is discussed based on the theory of Andreev reflection.

#024	MON	FAKT 1	15:00 – 15:15	HS 10

ASACUSA Cusp experiment

D. J. Murtagh[1] on behalf of the ASACUSA Cusp Collaboration

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The ASACUSA-Cusp experiment aims to perform spectroscopy of the hyperfine structure of antihydrogen by producing a beam of cold, spin polarized, ground state antihydrogen. The beam will be produced by mixing positrons and antiprotons in our unique Cusp trap which uses a pair of superconducting coils in an anti-Helmholtz configuration to produce a magnetic field capable of both confining the charged particles radially and polarizing the antihydrogen atoms.

Thus far, the collaboration has observed antihydrogen 2.7 m from the production region [1] and measured the distribution of principal quantum number of these atoms [2]. This weak beam was not suitable for the spectroscopy measurement so work commenced on improving the beam intensity and skewing the distribution towards ground state atoms. Simulations showed that the route towards this aim was producing colder dense positron plasmas [3].

Recently, a major technological milestone was achieved by the collaboration. Antihydrogen produced via three-body recombination will have an isotropic distribution, so a large open solid angle is needed for the antiatoms to escape. This has the disadvantage that the production region is illuminated by a hot (300 K) black body. Previously, it has not been possible to cool plasma below 130 K, however, a new electrode stack and coldbore with a focus on blocking microwaves from the room temperature region has allowed particles to cool to 25 K maintaining the large open solid angle for the beam to escape [4].

In this presentation I will discuss the methods used by the ASACUSA Cusp experiment and give details on the most recent work on plasma handling and beam production in the new Cusp trap.

[1] N. Kuroda et al., A Source of Antihydrogen for In-Flight Hyperfine Spectroscopy, Nat Commun 5, (2014).
[2] B. Kolbinger et al., Measurement of the Principal Quantum Number Distribution in a Beam of Antihydrogen Atoms, Eur. Phys. J. D 75, 91 (2021).
[3] B. Radics, D. J. Murtagh, Y. Yamazaki, and F. Robicheaux, Scaling Behavior of the Ground-State Antihydrogen Yield as a Function of Positron Density and Temperature from Classical-Trajectory Monte Carlo Simulations, Phys. Rev. A 90, 032704 (2014).
[4] C. Amsler et al., Reducing the Background Temperature for Cyclotron Cooling in a Cryogenic Penning–Malmberg Trap, Physics of Plasmas 29, 083303 (2022).

#025	MON	COND 1	15:15 – 15:30	HS 9

Investigation of magnetic and transport properties of intercalated transition metal dichalcogenides

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Transition metal dichalcogenides (TMDs) are layered materials that, due to their reduced dimensionality, host interesting phases such as charge density waves (CDW) and superconductivity. Owing to their layered structure, these materials can be intercalated with first-row transition metals. This suppresses CDW/superconducting ground states and while different magnetic orderings can form. They are attracting scientific attention also due to the possibility of exfoliation and various applications for new electronics and spintronic devices. We synthesized high-quality single crystals of Ni_xNbS_2 with a wide intercalation range ($0.01<x<0.6$), and stoichiometric $Co_{1/3}TaS_2$. We investigated the suppression of the parent compound SC state at low intercalations as well as the effect of disorder on the magnetic ground state in Ni_xNbS_2. It's interesting to notice that, while both compounds order antiferromagnetically, a ferromagnetic component also exists indicating the presence of Dzyaloshinskii-Moriya interaction. Alter magnetism is proposed recently in the $Co_{1/3}TaS_2$. Generally, the nature of those ground states is determined by the intercalated ion rather than the host material. Sometimes those magnetic orderings can be tuned by external parameters such as a magnetic field or hydrostatic pressure. We also performed ARPES to understand the impact of intercalation on the electronic structure near the Fermi level. Magnetotransport experiments and investigation of the impact of uniaxial pressure on the ground state are currently underway to gain a more comprehensive understanding of those materials and their electronic structures.

#026	MON	FAKT 1	15:15 – 15:30	HS 10

Study of Low Energy Antiproton Annihilations on Nuclei

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The antiproton-nucleus annihilation is one of the main processes in antimatter studies, as antiparticles are mostly detected through their annihilation. Despite its significance, the process itself is not well established and the lack of models for low energies complicates the simulation of detectors for the experiments conducted at CERN's Antiproton Decelerator.

A systematic study of antiproton-nucleus annihilations at 250 eV on a variety of thin foils is being set up at the ASACUSA facility. The target will be surrounded by a detection system using Timepix4 ASICs coupled to silicon sensors. A 3D reconstruction of the annihilation vertex from particle tracks in the single-plane detectors is not only used to tag individual events, but also to discriminate between antiprotons annihilating on the target and those scattering from it.

Therefore this experiment will provide data on minimum and heavily ionizing particle multiplicities from annihilations and the ratio of scattered antiprotons. This will enable a study of the possible final state interactions triggered by the primary annihilation mesons, as well as their branching ratios. The results will be implemented for assessment of simulation models such as the Liège Intranuclear Cascade model, and their potential tuning.

#027	MON	COND 1	15:30 – 15:45	HS 9

Reentrant Zero Resistance at Finite Magnetic Fields in Nanostructured Copper-Oxide Superconductor Films

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Zero resistance is one of the most known properties of superconductors. In type-II superconductors, such as copper-oxide superconductors, the absence of moving magnetic flux quanta is a prerequisite for a non-resistive state. Therefore, reentrant zero-resistance at a finite magnetic field is a strong indication of effective pinning of magnetic flux quanta.

As pinning centers, we introduce columns of point defects with suppressed critical temperature. We produce regular patterns of these defect columns by precisely positioning the focused beam of a helium ion microscope (He-FIB) on the surface of 30 to 50 nm thick superconductor films. The helium ions initiate collision cascades, displacing mainly oxygen atoms in the superconducting material while not affecting its crystal structure at an ion energy of 30 keV and moderate ion fluences.

Here, we present results of electronic transport measurements performed on nanostructured superconducting films: pronounced commensurability effects at magnetic fields as high as 6 T [1] and an ordered Bose glass behavior resulting from the interplay between pinning centers of different dimensionality [2, 3]. The strong pinning force of the artificial defects leads to reentrant zero resistance at a field of 3.8 T, and thanks to the precise arrangement of these defect columns, we can calculate the pinning force acting on a single flux quantum and its temperature dependence.

Acknowledgments. The research was funded by a joint project of the Austrian Science Fund (FWF), grant I4865-N, and the German Research Foundation (DFG), grant KO 1303/16-1. It is based upon work from COST Actions CA21144 (SuperQuMap), CA19140 (FIT4NANO), and CA19108 (Hi-SCALE) supported by COST (European Cooperation in Science and Technology).

References

1. M. Karrer et al., arXiv:2404.05382 (2024)
2. L. Backmeister et al., Nanomaterials, **12**, 3491 (2022).
3. B. Aichner et al., Condens. Matter 8, **32** (2023).

#028	MON	FAKT 1	15:30 – 15:45	HS 10

GRASIAN: Shaping and characterization of the cold hydrogen and deuterium beams for the forthcoming first demonstration of gravitational quantum states of atoms

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The antiproton-A low energy particle confined by a horizontal reflective surface and gravity settles in gravitationally bound quantum states. These gravitational quantum states (GQS) were so far only observed with neutrons, by Nesvizhevsky and his collaborators at ILL [1]. However, the existence of GQS is predicted also for atoms. The GRASIAN collaboration pursues the first observation of GQS of atoms, using a cryogenic hydrogen beam. This endeavor is motivated by the higher densities, which can be expected from hydrogen compared to neutrons, the easier access, the fact, that GQS were never observed with atoms and the accessibility to complimentary hypothetical short range interactions.
We report on our methods developed to reduce background and to detect atoms with a low horizontal velocity, which are needed for such an experiment. Our recent measurement results on the collimation of the hydrogen beam to 2 mm, the reduction of background and improvement of signal-to-noise and finally our first detection of atoms with velocities < 72 m/s are presented.

[1] V. Nesvizhevsky, H. Boerner, A. Petukhov, H. Abele, S. Baessler, F. Ruess, T. Stoferle, A. Westphal, A. Gagarski, G. Petrov, A. Strelkov, Quantum states of neutrons in the Earth's gravitational field. Nature 415, 297 (2002). https://doi.org/10.1038/415297a

#029	MON	COND 1	15:45 – 16:00	HS 9

Long-Term Stability and Annealing of Defects in $YBa_2Cu_3O_{7-\delta}$ Thin Films Produced with Collimated and Focused Helium Ion Beams

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$YBa_2Cu_3O_{7-\delta}$ (YBCO) thin films are modified by low-energy light-ion irradiation employing collimated and focused helium ion (He^+) beams and the long-term stability of irradiation-induced defects is investigated. The YBCO film resistance is measured in situ during and after irradiation and modeled. This reveals a strong influence of sample temperature on the formation and on the stability of the He^+ irradiation-induced defects. Thermal annealing experiments are performed to investigate the relaxation of irradiation defects. The activation energy for oxygen diffusion and re-arrangement into the YBCO unit cell basal plane is determined. The aging of YBCO thin films that are nanostructured into vortex pinning arrays via focused helium ion irradiation [1] is investigated by measuring resistivity and critical temperature and commensurability effects in magnetic fields. Interestingly, vortex matching effects do not deteriorate with sample storage time while the film resistivity shows some relaxation.

Acknowledgments
The research was funded by a joint project of the Austrian Science Fund (FWF), grant I4865-N, and the German Research Foundation (DFG), grant KO 1303/16-1. It is based upon work from COST Actions CA21144 (SuperQuMap), CA19140 (FIT4NANO), and CA19108 (Hi-SCALE) supported by COST (European Cooperation in Science and Technology).

References
[1] B. Aichner, B. Müller, M. Karrer, V.R. Misko, F. Limberger, K.L. Mletschnig, M. Dosmailov, J.D. Pedarnig, F. Nori, R. Kleiner, D. Koelle, W. Lang, “Ultradense tailored vortex pinning arrays in superconducting $YBa_2Cu_3O_{7-\delta}$ thin films created by focused He ion-beam irradiation for fluxonics applications”, ACS Applied Nano Materials 2 (2019) 5108−5115. https://doi.org/10.1021/acsanm.9b01006

#030	MON	FAKT 1	15:45 – 16:00	HS 10

Optimal operation of cryogenic calorimeters through deep reinforcement learning

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Cryogenic phonon detectors with transition-edge sensors achieve the best sensitivity to light dark matter-nucleus scattering in current direct detection dark matter searches. In such devices, the temperature of the thermometer and the bias current in its readout circuit need careful optimization to achieve optimal detector performance. This task is not trivial and is typically done manually by an expert. In our work, we automated the procedure with reinforcement learning in two settings. First, we trained on a simulation of the response of three CRESST detectors used as a virtual reinforcement learning environment. Second, we trained live on the same detectors operated in the CRESST underground setup. In both cases, we were able to optimize a standard detector as fast and with comparable results as human experts. Our method enables the tuning of large-scale cryogenic detector setups with minimal manual interventions.

#031	MON	COND 2	16:30 – 17:00	HS 9

Numerical analysis of many-body effects in cuprate and nickelate superconductors

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High-temperature unconventional superconductivity is arguably one of the most studied but least understood phenomena in solid-state physics. Indeed, the discovery of the first high-temperature superconductor, a copper oxide compound (cuprate), already dates back more than 35 years. Yet, there is no consensus concerning the mechanism behind superconductivity in those materials. Recently, also nickel oxide superconductors (nickelates), which are isostructural to cuprates, were discovered.

Here we analyze the electronic structure of both nickelates and cuprates and motivate the use of a single-band Hubbard model as a minimal description of the low-energy physics including superconductivity and the pseudogap. Despite its simplicity, the Hubbard model does not have an exact solution for arbitrary parameters. Hence approximate methods are needed, and we introduce the dynamical mean-field theory and dynamical vertex approximation (DGA) as methods of choice.

Using the DGA we analyze the real-frequency structure of the pseudogap and show that it can be understood as a 'momentum-selective insulator'. One of the key insights is that the Fermi surface, of the non-interacting case at the antinode, turns into a Luttinger surface (zeros of the Green's function). Fermi arcs, which are disconnected sections of the Fermi surface, appear as a result.

The last part of the talk reviews the superconducting dome of nickelate superconductors obtained using DGA plus a linearized Eliashberg equation for the superconducting eigenvalues. We extend this picture from infinite-layer nickelates to finite-layer ones and show that a correlation-driven charge transfer depletes the pockets derived from the rare-earth atoms and leads to `superconductivity without rare-earth pockets.

#032	MON	FAKT 2	16:30 – 17:00	HS 10

Aspects of General Relativity with Negative Cosmological Constant

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Solutions to general relativity with a negative cosmological constant have received significant attention due to the Anti-de Sitter/conformal field theory (AdS/CFT) correspondence — a conjecture which asserts that quantum gravity on Anti-de Sitter spacetimes is equivalent to a quantum field theory with conformal invariance in one dimension lower. While the AdS/CFT correspondence has been a successful tool to understand properties of a putative theory of quantum gravity, many questions regarding properties of the classical theory of gravity, general relativity, with a negative cosmological constant remain wide open to this day. In particular, it is not known whether the energy of solutions to general relativity with a negative cosmological constant is bounded from below. In this talk, I discuss properties of the energy of solutions to general relativity in two and three spatial dimensions. I discuss how gluing theorems provide constructive proofs of solutions to general relativity with certain properties. Finally, I will explain how such a gluing theorem can be used to show existence of solutions with negative scalar curvature, arbitrarily high genus and negative total mass in three spatial dimensions.

#033	MON	COND 2	17:00 – 17:15	HS 9

Non-relativistic Spin-splitting in Half-antiperovskite Collinear Antiferromagnets

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Antiferromagnetic materials, characterized by a net zero magnetization, have typically been viewed as having spin-degenerate energy bands, which confines them to passive roles in spintronics. However, recent theoretical predictions, supported by experimental observations, suggest that collinear antiferromagnets, depending on their specific magnetic symmetries, can break this spin degeneracy in momentum space, even in absence of spin-orbit coupling. This results in features analogous to those of ferromagnets (FMs). These materials, now called altermagnets, consist of spin-degenerate electronic states at the Γ point.

In this work, we systematically design twelve half-antiperovskite chalcogenides using density functional theory calculations. We first investigate their thermodynamic and dynamic stabilities, which are determined by evaluating the convex hull distance and phonon dispersion, respectively. Subsequently, the magnetic ground-state analysis reveals that a collinear antiferromagnetic structure has the lowest energy. We then calculate the band structures and investigate the spin-splitting of the energy bands. Based on magnetic symmetries, we examine the reasons behind the spin-degeneracy of energy bands at some high-symmetry points and spin-splitting at others. Our findings advance the understanding of the crystal and magnetic structures of half-antiperovskites, paving the way to further explore these materials for antiferromagnetic spintronic applications, which is corroborated by our observations of spin-splitting phenomena.

#034	MON	FAKT 2	17:00 – 17:15	HS 10

Carroll black holes

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Despite the absence of a lightcone structure, some solutions of Carroll gravity show black hole-like behaviour. We define Carroll black holes as solutions of Carroll gravity that exhibit Carroll thermal properties and have a Carroll extremal surface, notions introduced in this talk. The latter is a Carroll analogue of a Lorentzian extremal surface. As examples, I discuss the Carroll versions of Schwarzschild and black hole solutions of generic 1+1 dimensional Carroll dilaton gravity like Carroll JT black holes.

#035	MON	COND 2	17:15 – 17:30	HS 9

Reentrant normal phase in superconducting NbN layers and magnetic proximity effect

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At the interface between a ferromagnet (FM) and a superconductor (SC), a plethora of emergent quantum phenomena, such as spin triplet superconductivity, gapless superconductivity and topological superconductivity, emerge due to a synergy between superconducting and magnetic order. By combining macroscopic quantum interference with microscopic exchange interactions, spin selectivity and spin transport, such proximity induced effects in SC/FM heterostructures have emerged as the basis for both fundamental physics and quantum devices including magnetic Josephson junctions, superconducting diodes, quantum sensors and detectors.

Here, we report on the effect of underlying ferromagnetic Fe_4N nanocrystals (NC) on the superconducting properties of epitaxial NbN thin layers. Thin NbN epitaxial layers of thickness 20 nm are grown on epi-ready *c*-Al_2O_3 substrate and on GaN:Si(130 nm)/Fe_4N NC/ *c*-Al_2O_3 templates using a plasma enhanced atomic layer deposition (PE-ALD) system. The grown samples are characterized by x-ray diffraction, x-ray photoelectron spectroscopy, transmission electron microscopy and low-*T*/high-$\mu_0 H$ magnetotransport. The magnetotransport studies are performed in a van der Pauw configuration using a phase locked lock-in *ac* technique. The superconducting transition temperature T_c for NbN/*c*-Al_2O_3 and for NbN/GaN:Si(130 nm)/Fe_4N NC/*c*-Al_2O_3 are recorded to be 14 K and 13.2 K, respectively. This lowering of the T_c is attributed to the magnetic proximity effect (MPE). A reentrant resistive state with a peak feature in the Hall resistivity is recorded for the NbN/GaN:Si(130 nm)/Fe_4N NC/*c*-Al_2O_3 case and is attributed to the pinning of the vortices due to the underlying Fe_4N nanomagnets. This peak Hall resistivity is also shown to be tunable as a function of *T* and $\mu_0 H$. The MPE reported in this work is exected to find applications in nitride based superconducting spintronics.

#036	MON	FAKT 2	17:15 – 17:30	HS 10

Hadronic light-by-light contributions to the muon g-2 in holographic models of QCD

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The Standard Model calculation of the anomalous magnetic moment of the muon suffers from uncertainties due to the non-perturbative nature of QCD. After the hadronic vacuum polarisation diagrams the second most important contributions are light-by-light scattering diagrams. We present computations of transition form factors, which are key ingredients in the light-by-light analysis, using an alternative string theory inspired approach called holography. We compare our results to existing lattice and experimental data which are rather well reproduced due to the chiral anomaly. We comment on the importance of short distance constraints and the role of axial vector mesons and provide a way to include strange quark mass and axial anomaly effects. Finally we discuss improvements and generalizations of our current models.

#037	MON	COND 2	17:30 – 17:45	HS 9

Waterfalls: umbilical cords at the birth of Hubbard bands

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Waterfalls are high-energy anomalies in an angle-resolved photoemission spectrum characterized by a steep drop of momentum-energy dispersion, typically identified using momentum distribution curves (MDCs), and a significantly smeared spectrum. These anomalies have been frequently observed in cuprates [1-3], and more recently in superconducting nickelates [4,5], with the onset of the waterfall occurring at around 100-200 meV and extending up to approximately ~1eV.

Here we argue that such anomalies naturally emerge within the Hubbard model when a Hubbard band develops and separates from the quasiparticle band. We demonstrate this by treating the electronic correlations on the level of dynamical mean-field theory. To draw an analogy with experimental analysis, we also calculate the second derivative of the MDCs. The corresponding second derivative spectra, even more clearly than the bare spectra, highlight the waterfall structure within our calculations.

Finally, we compare our results for the Hubbard model with the *ab initio* determined parameters with the measured spectra in cuprates and nickelates for various levels of hole doping. Our findings show a good agreement between the theoretical predictions and experimental observations.

[1] B. P. Xie *et al*., Phys. Rev. Lett. 98, 147001 (2007).
[2] T. Valla *et al*., Phys. Rev. Lett 98, 167003 (2007).
[3] W. Meevasana *et al*., Phys. Rev. B 75, 174506 (2007).
[4] W. Sun *et al*., arXiv:2403.07344 (2024).
[5] X. Ding *et al*., arXiv:2403.07448 (2024).

#038	MON	FAKT 2	17:30 – 17:45	HS 10

Complex Langevin simulations with a kernel

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Quantum Chromodynamics (QCD) is the theory describing the strong interactions between quarks and gluons that lead, for instance, to the formation of protons and neutrons that make up atomic nuclei. To date, the most successful tool for the study of QCD beyond perturbation theory is lattice quantum field theory. However, conventional lattice field theory methods (based on importance sampling) are not applicable within the finite-baryon-density regime of QCD, which is, e.g., relevant for our understanding of compact stellar objects such as neutron stars. This failure is due to the infamous sign (or complex action) problem.

In this talk, I will discuss the so-called *Complex Langevin* method as an alternative to the conventional approach. The underlying idea is a complexification of the relevant degrees of freedom, which can – in principle – be used to overcome the sign problem. However, as I will outline, this complexification does not come without problems, as it may in some cases lead to diverging simulations or – even worse – convergence to wrong solutions. I will discuss the possible origins of these drawbacks and how they – in particular the latter – may be overcome via the introduction of a so-called *kernel* into the Complex Langevin formalism.

#039	MON	COND 2	17:45 – 18:00	HS 9

Murunskite: a bridge between cuprates and pnictides

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Despite exceptional scientific efforts over several decades, there is almost no universal agreement about the superconducting state of cuprate compounds. A constructive way to improve understanding would be to synthesize and investigate a new system, which displays superior chemical flexibility and tunability of the valence of the transition metal ions. One could then manipulate its various electronic, metallic, and mechanical properties. We study murunskite, which interpolates between cuprates and pnictides[1]. This presentation will report the successful growth and characterisation of the first-ever high-quality Murunskite single crystals. These crystals show semiconductors like the parent compounds of cuprates, yet isostructural to the metallic iron-pnictides. Moreover, like both families, it has an antiferromagnetic response with an ordered phase below 100 K. Spectroscopy (XPS) and Density Functional Theory (DFT) calculations concur that the sulfur 3*p* orbitals are partially open, making them accessible for charge manipulation, which is a prerequisite for superconductivity in analogous layered structures. Furthermore, DFT indicates that the valence band is more cuprate-like, while the conduction band is more pnictide-like. We also managed to substitute Fe with Co in the parent compound, leading to superconductivity in this family for the first time.

[1] D.Tolj, et al, Applied Materials Today, Volume 24, 101096, (**2021)**

#040	MON	FAKT 2	17:45 – 18:00	HS 10

An exciting hint towards the solution of the neutron lifetime puzzle?

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We revisit the neutron lifetime puzzle, a discrepancy between beam and bottle measurements of the weak neutron decay. Since both types of measurements are realized at different times after the nuclear production of free neutrons, we argue that the existence of an excited state could be responsible for the different lifetimes. We elaborate on the required properties of such a state and under what circumstances it is possible that it has not been experimentally identified yet.

#041	TUE	YM 1	14:00 – 14:30	HS 8

In Berührung mit Drogen

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Nehmen Sie an diesem Science Slam teil, und entdecken Sie den tiefen Zusammenhang zwischen Pharmazie und Physik sowie die vielfältigen Möglichkeiten, wie man sich als Physiker damit beschäftigen kann.

Im Laufe des Science Slam werden Sie lernen, wie man Nanopartikeln ganz einfach herstellt und sogar aus der eigenen Alltag kennt. Dabei wird deutlich gemacht, warum Nanopartikeln eine wichtige Rolle in der medizinischen Behandlung spielen. Danach werden Sie sehen, wie Sie die Nanopartikeln durch Beleuchtung und Berührung messen. Einerseits können Sie Nanopartikeln in Flüssigkeit durch die Streuung von Licht erkennen, aber um jede einzelne Nanopartikel zu messen reicht das nicht aus. Deswegen benutzt man auch Rasterkraftmikroskopie, in dem eine Nanospitze die Nanopartikeln abtastet um ein Bild von ihnen zu erstellen. Mutige Teilnehmern können dies selbst erleben, in dem sie zu einem Rasterkraftmikroskop in größerem Maßstab werden.

Schließlich werden Sie sehen, aus was biologische Zellen bestehen, und warum sie einerseits eigentlich sehr ähnlich zu Federn sind. Sie werden ebenso selber entdecken, wie man als Physiker damit umgeht, wenn die Zellen doch etwas von idealen Federn abweichen. Alles einfach damit wir den Effekt von Arzneistoffen erkennen.

Am Ende des Science Slams haben Sie hoffentlich Spaß gehabt und vielleicht sogar eine bessere Vorstellung davon mit welcher Physik Sie sich selber beschäftigen möchten.

Sie sind alle sehr willkommen!

#042	TUE	YM 1	14:30 – 15:00	HS 8

AI-Driven Innovations in Physics and Material Science: Selected Examples

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Artificial Intelligence (AI) is increasingly being used in the field of material science and has been instrumental in various fields of physics. In astronomy, for example, artificial neural networks can plow through mounds of data with little to no human input, highlighting abnormalities and recognizing patterns that humans would never have noticed. AI can speed up the discovery and development of materials by a factor of 10 to 100. While most examples are based on large volumes of data, AI can also be helpful when little data is available.

We use machine learning to predict the mechanical properties of WC-Co cemented carbides, also known as hardmetals, from magnetic data only. Useful for geophysics is the identification of magnetization states in sediments. We have demonstrated the principal possibility of such an identification based on machine learning in large-scale nano-ellipses arrays. Another example is the predictive maintenance for ball bearings in manufacturing industry. Here, the tables are turned: physics and simulations help to train an AI model. Furthermore, reinforcement learning can be used to optimize air conditioning in buildings and helps with predictive maintenance. The green energy transition is not possible without permanent magnets. We do AI-supported development of hardmagnetic materials for electric motors in e-cars, wind turbines, etc.

#043	TUE	YM 1	15:00 – 15:30	HS 8

Measurement of ion residence times in the ILIAMS cooler with a new multi-beam switcher

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The ILIAMS (Ion-Laser InterAction Mass Spectrometry) ion cooler, developed at VERA (Vienna Environmental Research Accelerator), plays a pivotal role in providing accelerator mass spectrometry of long-lived radioisotopes at environmental levels. By combining a gas-filled RFQ ion guide with high-powered lasers, ILIAMS suppresses unwanted isobaric anions, which are typically orders of magnitude more abundant than the isotope of interest, via laser photodetachment. The suppression efficiency is limited by the ion residence time inside the cooler, which can be varied mainly through the buffer gas pressure and the guiding field strength. So far, the ion beam has been injected into the cooler using a dipole magnet, which prohibits fast switching between the injected ion species.

As part of the master thesis presented in this talk, simulations aided in the design and construction of a new multi-beam switcher (MBS). The application of a voltage of up to 5 kV to the electrically insulated vacuum chamber inside the magnet leads to an acceleration and thus, a modified deflection angle of the ions, allowing switching between closeby masses within tens of µs.

For the first time, measurements of the ion residence time distribution at equilibrium conditions were performed using the MBS. Through sequential injection of the stable isotopes $^{35}Cl^-$ and $^{37}Cl^-$, followed by mass separation by a Wien filter, the buildup- and washout functions of both ion species were observed. These experiments both yielded data on the equilibrium residence time distribution as well as a first-time direct observation of space charge effects: The about 3-times higher-current $^{35}Cl^-$ beam pushed the previously injected, lower-current $^{37}Cl^-$ ions through the cooler, yielding a peak in the washout function. This allowed for a direct quantification of space charge effects inside the ILIAMS cooler, which propagated through the cooler 4 to 10 times as fast as the ions themselves.

#044	TUE	YM 2	16:00 – 16:30	HS 8

Low energy effective description of light pseudo-scalar mesons in SO(N)-like dark QCD

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Dark matter (DM) is one of the most prominent mysteries in modern physics. Recently, theories of strongly interacting massive particles (SIMPs) gained a lot of attention as explanation for DM at the level of particle physics. This class of theories features strong self-interactions among the DM particles, resolving the cusp vs. core problem and offers an explanation for the stability of DM. In my master thesis, I investigated realizations of SIMP dark matter through non-Abelian gauge theories with two Dirac fermions transforming under a real representation of the gauge group. The lightest stable states, relevant for phenomenology of cold DM in the late universe, were studied by applying chiral effective field theory methods consistently combined with a large N expansion. As the result of this work, I identified the relevant physical degrees of freedom for DM phenomenology and provide an effective Lagrangian that allows to study processes among them at non-relativistic energies. The topological terms of Wess-Zumino type, dominating the production mechanism of DM via freeze-out, have been classified and explicitly calculated. Due to the non-trivial geometry of the coset space SU(4)/SO(4), standard technique was unreliable in this case and more modern approaches were used. Furthermore, we discuss the introduction of a dark photon portal between the dark and visible sector and some consequences on the DM stability. Connections to the underlying gauge theory are provided, which allow to study these theories via non-perturbative methods like lattice field theory in the future.

#045	TUE	ENS	16:00 – 16:15	HS 9

Thermoelectric Waste Heat Recovery: Materials, Modules & Applications

C. Beisteiner[1], L. Gupfinger[2,3], C. Scherner[2,3], P. Zellinger[2,3], O. Maier[3], and K. H. Gresslehner[2,3]

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In this presentation the current status of materials research, module production and applications of thermoelectricity (TE) - focused on thermal energy conversion - will be discussed.

Waste thermal energy is a by-product in every power generation and industrial processes. It is one of the largest sources of inexpensive, clean, and fuel-free energy available. Thermoelectric generators (TEG) had been demonstrated to be a promising technique that can convert any form of waste heat directly into higher-value electrical energy. TEG are solid-state devices that use the Seebeck effect, with the advantages of having no moving parts, no working fluids, easy scalable, low maintenance costs, noiseless operation and a long life-span.

From application point of view, TE materials used in TE modules, can roughly grouped into three categories attending to their temperature range of operation.

In the low- and mid-temperature range (i.e. 350 K – 600 K) the well-researched Bi_2Te_3-based materials are used almost exclusively. Therefore, thermoelectric modules are available on the market and can be used for many applications such as energy recovery systems, medical applications, body heat, measuring and transmitting sensor data e. g. for IoT applications, etc. as well as for cooling purposes.

At moderately high temperatures (i.e. 500–900 K) materials based on IV-VI compounds such as PbTe, $Pb_{1-x}Sn_xTe$, GeTe or SnTe were typically used. Due to the Pb ban and the low abundance of the chemical element Te the production of PbTe-based modules was discontinued worldwide. Currently, promising TE materials for this temperature range are Skutterudites, Half Heusler alloys and SnSe compounds which are used for industrial energy recovery systems, automotive applications, etc.

For high-temperatures applications (>900 K) such as recovery of waste radiant heat e. g. in the steel industry, etc., providing electricity in spacecrafts, typically $Si_{1-x}Ge_x$ ($x \approx 0{,}2$ - $0{,}6$) alloys were used.

#046	TUE	GEP	16:00 – 16:15	HS 10

Various historical balances

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A selection of special balances from the historical physics collection of the University of Vienna will be presented. In principle, these experimentally tested objects still work quite well. In 1894 Ludwig Boltzmann purchased a universal precision balance from J. Nemetz. It is characterised by an ingenious external weight support. An analytical balance from Starke & Kammerer (ca. 1925), has a fascinating external fraction gram support as well. The demonstration balance from Alb. Rueprecht & Sohn for lecture experiments, dating from around 1910, is also noteworthy. The Mohr balance and a decimal balance were also purchased around 1910. Thomson's absolute plate electrometer dated 1882 compares electrostatic force and weight force. Measurement results are also shown and discussed for the Hartmann & Braun current balance (ca. 1894) and the Waltenhofen balance from Franz Steflitschek (1888).

#047	TUE	LHS	16:00 – 16:15	BA 9911

Error culture in STEM lessons: The connection between the nature of science and dealing with errors

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Numerous studies and research findings in recent years have shown that dealing with errors appropriately can significantly improve students' learning (Metcalfe, 2017). Errors are not only of great importance in the school context, but also in the acquisition of scientific knowledge. They enable a better understanding of how scientific knowledge is created. Errors are therefore essential components of the so-called 'Nature of Science' (NOS), i.e. the understanding of how science works (Allchin, 2011).

This study provides the first empirical results on the relationship between the understanding of NOS aspects and dealing with errors in the context of STEM lessons. Among other things, it was investigated to what extent pupils' understanding of NOS aspects influences the way they deal with errors. To answer this research question, the pupils were surveyed using a questionnaire. The sample consisted of 269 pupils from German-speaking Switzerland (7th-9th grade). The results show that the understanding of NOS aspects has an influence on error learning orientation. The results also show that the effect of understanding NOS aspects on affective-motivational reactions to errors is mediated by error learning orientation.

These findings suggest that the topic of errors should be given greater importance in the context of NOS. The results of this study therefore not only contribute to the scientific understanding of NOS, but also have concrete implications for educational practice, particularly in the area of science education.

References

Allchin, D. (2011). Evaluating knowledge of the nature of (whole) science. Science Studies and Science Education, 95(3), 518-542. doi:https://doi.org/10.1002/sce.20432

Metcalfe, J. (2017). Learning from Errors. Annual Review of Psychology, 68, 465-489. doi:https://doi.org/10.1146/annurev-psych-010416-044022

#048	TUE	OGD 1	16:00 – 16:15	BA 9910

Melt Memory Effect of a Benzothienobenzothiophene Derivative

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The class of benzothieno-benzothiophene (BTBT) molecules attracts large attention, since it shows outstanding performance organic thin film transistors. One specific derivative of BTBT type molecules in the one with oligoethylene-side chains attached at the terminal end of the conjugated core. A classical polymorph screening procedure is performed to examine the variety of polymorph phases of this molecule. Two polymorph phases and one solvent with dichloromethane was found. Expanding the methodology towards crystallisation at surfaces reveal the same polymorphs but additional four unknown solvents; three solvates with dichloromethane and one solvent with dichlorobenzene. A number of experimental techniques are used to probe the bulk properties of the solvates including grazing incidence X-ray diffraction, X-ray fluorescence and Raman spectroscopy. Temperature dependent experiments – i.e. hot stage microscopy and X-ray diffraction - reveal an interesting melt memory effect. Starting from a specific solvent and heating the solvate above the melting temperature and above the optical clearance temperature and cooling down to room temperature result in the crystallisation in the same specific solvate of the melting procedure. Only at temperatures 50 K above the melting temperature and 20 K above the clearance temperature the melt memory is lost and the stable polymorph is formed. The underlying mechanism for the melt memory is explained by a strong interaction of the solvent molecule dichloromethane with the oligoethylene side chains of the molecule. While melt memory is widely known for polymers such effects are hardly observed for molecular crystals. Generally, the suggested mechanism has to be considered for thin film preparation by solution processing.

#049	TUE	ENS	16:15 – 16:30	HS 9

Modular heat pump system with natural refrigerant as a replacement for gas boilers in multi-family houses

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Despite the uncertain supply situation and short-term price shocks, natural gas remains the largest primary energy source for heating and cooling in Europe. In large cities such as Vienna, around half of all households continue to use gas boilers for heating or domestic hot water preparation. On the way to a climate-neutral city the transition from gas to environmentally friendly heat pumps is unavoidable – also for large multi-family houses. The FFG-project "Gasthermenersatz" aims to solve this problem by developing a functional model of a decentralized, sound-optimized heat pump solution.

The innovative solution consists of series- and parallel-connected refrigeration circuit modules. Depending on the interconnection of a certain number of such hermetically sealed refrigeration circuit modules, the resulting heat pump is a drop-in alternative to the gas boiler in large multi-family houses. In operational use, access to the heat source is crucial and obtained either from the outside air or geothermal heat. Both can be connected to the heat pump system via the now unused chimney. The temperature level of the installed heating system should be reduced to maximize the efficiency of the heat pump. Still, the impact on the installed heating system can be minimized with market available solutions if the overall heating demand of the building is decreased by improving the insulation of the building.

The results include a laboratory validated and tested concept of a novel decentralized heat pump. In addition, the analysis is supported via log(p),h-diagrams, which allow to illustrate the design of the system. To compare this solution with other concepts or heat pumps, the seasonal coefficient of performance is calculated.

A successful implementation of the concept will lead in the medium term to a holistically optimized, highly efficient technical solution for providing heating, cooling and hot water as an alternative to gas boilers in densely populated urban areas.

#050	TUE	GEP	16:15 – 16:30	HS 10

Traces of Transfer Matrix and Potts Model in Ising's Thesis

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In his dissertation from 1924 Ernst Ising calculated the partition function of several one-dimensional models in the hope to prove the existence of a ferromagnetic phase. As he actually only considered a one-dimensional model, he did not succeed in proving ferromagnetism, but he was able to calculate the partition function for this case of the 2-state model, now called the Ising chain, exactly. The crucial result of his calculations is a polynomial whose largest root defines the partition function in the thermodynamic limit. While this result has been published, extensions to this chain that he made in his dissertation have been only mentioned but not explained.

It is pointed out that Ising's polynomial corresponds to the characteristic polynomial of the transfer matrix later found within the solution of the spin model. The extensions he made are discussed in the light of this connection. He calculated this polynomial for a 3-state model – an unknown precursor to the Potts model.

Ising also tried to extend his model to two chains, but did not consider the interaction between the chains. On the other hand, he looked at the effect of an additional next-nearest neighbor interaction for the magnetization. His results are discussed in the light of later work for these cases. Since in all these cases the characteristic polynomial is of higher than second order, an exact solution was not possible for Ising and he could not find an analytic solution without approximations.

#051	TUE	LHS	16:15 – 17:30	BA 9911

Session der Sektion Physik und Schule (LHS)

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Preisträgervorträge der VWA-Preisträgerinnen und -Preisträger der ÖPG2024
Dauer: 10 Minuten pro Preisträger:in
Schülerinnen und Schüler können ihre Vorwissenschaftlichen Arbeiten im Unterrichtsfach Physik bei der ÖPG einreichen. Im Jahr 2024 gab es 79 Einreichungen, aus denen 5 Preisträgerinnen und Preisträger ermittelt wurden.

Vorstellung des IYPT Tournament
Dauer: 15 Minuten
Das österreichische Team des International Young Physicists' Tournament präsentiert seine Beiträge. Das IYPT zeichnet sich durch Teamarbeit bei der Präsentation von Lösungen physikalischer Aufgaben aus. Der Beitrag wird in englischer Sprache gehalten.

Vorstellung der Physikolympiade
Dauer: 15 Minuten
Bei der internationalen Physikolympiade treten Schülerinnen und Schüler gegeneinander an, um theoretische und experimentelle Aufgaben zu lösen. Die diesjährigen Teilnehmenden geben einen kurzen Einblick.

Anmerkung:
Die Teilnahme an der Veranstaltung Physik und Schule ist auch ohne Entrichtung der Teilnahmegebühr für die ÖPG-Tagung möglich. Bitte schreiben Sie eine E-Mail mit den Namen der Personen, die kommen möchten, an: oepg@physikdidaktik.info

#052	TUE	OGD 1	16:15 – 16:30	BA 9910

Transient absorption microscopy to investigate higher excitations of Squaraines

R. Schwarzl[1], M. Jeindl[1], M. Schiek[2,3], N. Taghizade[4], A. Windischbacher[4], P. Puschnig[4], F. C. Spano[5], D. Giavazzi[6], A. Painelli[6], and M. Koch[1]

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Transient absorption is an established technique for investigating ultrafast behaviour in optically dense materials. We employ its spatially resolved variant, transient absorption microscopy, in order to investigate the temporal behavior in a class of organic, quadrupolar molecular crystals, Squaraines. Their optical properties in the visible to the near IR result from exceptionally strong intermolecular coupling which follows a pronounced structure-function relationship, making it possible to adapt optical properties by the adjustment of molecular packing. While the optical properties in equilibrium have been studied in-depth, time-resolved dynamics of Squaraines on femtosecond time scales have only recently started to emerge.

I will present transient absorption results in an orthorhombic Squaraine together with measurements of a solid solution, thereby comparing strongly coupled and dilute molecules. These experimental results will be complemented to ab-initio and semi-empirical approaches aimed at determining the spectral and polarization properties of higher excited states which are beyond the reach of conventional spectroscopy techniques.

#053	TUE	ENS	16:30 – 16:45	HS 9

Experimental characterisation of the charge and discharge behaviour of a PCM storage

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The latent heat storage realised within the Horizon Europe HYPERGRYD project is a cuboid heat exchanger, containing phase change material (PCM) within a metallic structure made out of aluminium. This heat exchanger operates with water with corrosion inhibitor as heat transfer fluid on both the charging as well as the discharging side, whereas the PCM is embedded in the fins. Four such heat exchangers in parallel operation form the PCM storage. It is charged by hot water from the condenser side of a heat pump system. Then, the heat is transferred inside the storage to the PCM, which is first heated sensibly until its melting point and subsequently melts. Later, the storage is discharged via water to meet the demand for domestic hot water (DHW) applications. The PCM storage material utilized is RT57HC, which was chosen because of its high storage capacity and specific heat capacity.

The sensors used to evaluate the system behaviour were PT-1000 thermocouples installed at the in-let and outlet of the PCM storage modules. For the measurement of the mass flowrate, a Coriolis mass flow meter was installed. On the discharge side, two more PT-1000 thermocouples were present to measure the temperatures. The operating modes being tested were different water mass flow rates, simulating different conditions of DHW supply – 4.8 kg/min for showering with low flow rate or with an eco-showerhead and 10.1 kg/min for showering with a larger flow rate. The mass of the water exiting the discharge line was measured using a scale.

When feeding the discharge line with water with a temperature of 15°C and a mass flow rate of 4.8 kg/min, the discharge outlet temperature reaches a peak of about 60°C after around 1 minute, which corresponds to a rapid response time. During the following 11 minutes, the outlet temperature remains above 55°C, therefore showing the capability to provide high temperatures for a prolonged amount of time sufficient for an average showering process.

#054	TUE	GEP	16:30 – 16:45	HS 10

Wurmprecht's eclipse predictions for the years 1373 to 1386

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In ancient times eclipses of the sun and the moon were seen as very important celestial phenomena, and therefore, they played an important role in the astronomy of early cultures.

Stift Rein, the oldest still existing Cistercian monastery, situated in the North of Graz, contains some interesting astronomical manuscripts, among them is CodRun 204, the so-called Wurmprecht calendar. This is one of the oldest calendars written in German language. As stated in the accompanying text the calendar was written by Wurmprecht in Vienna and dated to 1373. It is interesting that the name Wurmprecht doesn't show up in any other manuscripts.

In addition to an eternal calendar Wurmprecht gives several astronomical, religious, and astrological information, for example a prediction of solar and lunar eclipses for the years 1373 to 1386. The solar and lunar eclipse predictions are followed by a table to calculate the position of the moon in the respective constellation, a table of the regents by the hour and tables to calculate the time between Christmas and Carnival Sunday, dominical letters and the golden number, finally a text for fortune telling using the position of the moon in the zodiac.

In this presentation Wurmprecht's predictions of solar and lunar eclipses will be presented and described in detail. His way of predicting eclipses will be compared with descriptions of other manuscripts of that time and with descriptions in the literature. The accuracy of Wurmprecht's predictions will be compared with data from the catalogue of solar and lunar eclipses from NASA. Furthermore, details like, for example concerning saints of the respective day of the eclipse, will be compared with information in the calendar.

#055	TUE	OGD 1	16:30 – 16:45	BA 9910

Significance of Charge Transfer Excitons for Giant Excitonic Circular Dichroism

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Quadrupolar anilino squaraine dyes exhibit distinct excitonic signatures in their visible absorption spectra due to strong intermolecular interactions. These excitons are a result of the spatial arrangement of the molecular backbones, which is steered by non-chromophoric terminal functionalization patterns. They can be of predominantly Frenkel-excitonic nature [1] or are hybridized with intermolecular charge transfer [2] and may feature an extraordinary strong excitonic circular dichroism [3] especially in aggregated thin films [4]. Theoretical modeling with a modified essential state model based on true magneto-electric CD finds two possible scenarios for dispersed colloidal aggregates: two concomitant aggregate species or a single aggregate type involving intermolecular charge transfer [4]. Finally, transient absorption spectroscopic investigations on thin films give unambiguous insights into the excitonic nature of aggregated thin films [5].

[1] Balzer, Breuer, Witte, Schiek. Template and Temperature-Controlled Polymorph Formation in Squaraine Thin Films. Langmuir 38 (2022) 9266.
[2] Balzer, Hestand, Zablocki, Schnakenburg, Lützen, Schiek. Spotlight on Charge-Transfer Excitons in Crystalline Textured n-Alkyl Anilino Squaraine Thin Films. J. Phys. Chem. C 126 (2022) 13802.
[3] Schulz, Zablocki, Abdullaeva, Brück, Balzer, Lützen, Arteaga, Schiek. Giant Intrinsic Circular Dichroism of Prolinol-Derived Squaraine Thin Films. Nat. Commun. 9 (2018) 2413.
[4] Gavazzi, Schumacher, Grisanti, Anzola, Di Maiola, Zablocki, Lützen, Schiek, Painelli. A Marvel of Chiral Squaraine Aggregates: Chiroptical Spectra beyond the Exciton Model. J. Mater. Chem. C 11 (2023) 8307.
[5] Bernhardt, Rieland, Wang, Schumacher, Lützen, Schiek, Loosdrecht. Insights from Transient Absorption Spectroscopy … to be published (2024).

#056	TUE	ENS	16:45 – 17:00	HS 9

Design and Characterization of a High Temperature Heat Pump with Ejector

L. Stöger[1,2], M. Schieder[1], C. Illich[3], T. Königsecker[3], M. Mair[3], J. Unterluggauer[1], S. Kling[1], V. Sulzgruber[1], A. Stingeder[3], M. Lauermann[1], T. Ciepiela[3], C. Reichl[1, 4]

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Heat pumps offer a highly efficient alternative to fossil fuels like coal and gas by utilizing waste heat with minimal use of electricity. Industrial heat pumps are especially pertinent to the manufacturing sector. However, in the expansion valves used in traditional heat pumps an irreversible dissipation process occurs.

An innovative component inserted into the refrigeration circuit, the ejector, has the potential to decrease these losses significantly and improve the Coefficient of Performance of heat pumps by up to 26% in comparison to conventional systems.

An ejector normally is a passive component without moving parts consisting of three openings – the suction, motive and outlet nozzle: The high-pressure motive flow induces a suction flow from the low-pressure side, resulting in a higher pressure at the compressor inlet. This process reduces the electrical power required for compressor operation.

Within the FFG's research project “ETHP – Ejector Technologies for Heat Pumps”, an industrial high-temperature heat pump featuring an ejector was designed. The system was optimized for a source temperature of approximately 45°C and a sink temperature of around 130°C. Various ejector geometries were simulated and compared until an optimal ejector design with a variable inner geometry was identified.

The heat pump and ejector were manufactured and put into operation. Over 30 sensors were installed to gather measurement data on pressure, temperature gradients, and refrigerant mass flow at various points within the refrigerant circuit. The collected data were analyzed and visualized in real-time using LabVIEW, focusing particularly on the impact of the ejector. The data provide the foundation to validate the three-dimensional simulation models of the ejector.

#057	TUE	GEP	16:45 – 17:00	HS 10

Development of radio science investigations in Austria

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In 1890 Ernst Lecher studied resonance phenomena including those related to radio wave propagation. Starting in 1903 Max Reithoffer regularly delivered lectures on "electrical oscillations/waves" at the Polytechnical Institute in Vienna. In 1904 Otto Nußbaumer could already transmit music within the Polytechnical Institute building in Graz.

One of the most ambitious scientists/engineer of the "second generation" was Heinrich Löwy (1894-????), born in Vienna, educated at Universities of Vienna and Göttingen (Germany), who studied electromagnetic wave propagation for investigations of the Earth's interior and geophysical prospection, even from balloons and airplanes.

In the 1930ies the first investigators of the ionosphere by electromagnetic waves were Josef Fuchs (1904-1989) and Otto Burkard (1908-2015). Fuchs was first investigating different ionospheric parameters and afterwards developed methods to measure heights and distances by radio waves. Burkard was the first after WW2 to establish an ionosonde at the University of Graz to characterize the ionosphere and thereby laid the ground for a "small school of radio science", among the members were many later expatriates, e.g. Willi Nordberg (1930-1976), Siegfried J. Bauer (1930-), Gernot M.R. Winkler (1922-2016), who worked in the United States of America.

End of the 1960ies another line of investigations was established by Ernst Ledinegg (1910-2004), specializing in waveguide propagation, and Willibald Riedler (1932-2018), studying terrestrial but also space radio wave propagation, at the University of Technology Graz.

In the 1990ies and beyond two other research groups, both at the Space Research Institute of the Austrian Academy of Sciences, were established in Graz. One by Helmut O. Rucker, focusing on radio physics at the outer planets and the Sun, the second by Konrad Schingenschuh, investigating "Schumann resonances" at other planets and moons, as well as starting investigations in the field of seismo-electric activities and its relations to the ionosphere.

#058	TUE	OGD 1	16:45 – 17:00	BA 9910

Thermal stability of MBE and CVD grown GeSn layers: in situ TEM investigation

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$Ge_{1-x}Sn_x$ alloys are of great interest due to their property of tunable band gap depending on the Sn concentration. It has been found that a transition to a direct band gap can be achieved when Sn concentration exceeds 6 at% [1], making these alloys optimal for Si-based electronics and optoelectronics. However, the low solubility limit reduces the thermal stability of GeSn alloys, resulting in Sn segregation [2]. Therefore, studying thermal stability is essential for predicting the thermal budget to which a $Ge_{1-x}Sn_x$ layer can be exposed during device fabrication.

The technique of *in situ* transmission electron microscopy (TEM) allows studying the dynamic process during thermal annealing experiments. With this technique, we analyze how the Sn concentration and the presence of dislocations affect the thermal stability [3]. In this regard, samples grown by CVD and MBE, 50 nm thick epilayers with 6-14 at% Sn, were analyzed in cross-section and plan-view geometries. The lamellae were cut and installed on micro-electro-mechanical system (MEMS) heating chips with a focused ion beam (FIB).

For the MBE samples, two different concentrations of 10 and 14 at% Sn were investigated, showing stability up to 500°C and 350°C, respectively. Sn-based precipitates are formed at these temperatures, exhibiting β-Sn crystal structure, determined by high-resolution TEM and Fast Fourier transform (FFT) analysis. In the case of the CVD samples, the studied concentrations were 6 and 11.5 at% Sn, forming Sn precipitates at 650°C and 450°C, respectively. The results show the highest stability for the sample with 6 at% Sn and the lowest for the sample with 14 at% Sn, which indicates a strong dependence of the decomposition temperature on the Sn content regardless of the growth technique.

[1] J. Doherty *et al.*, *Chem. Mater.*, vol. 32, no. 11, 2020

[2] A. Minenkov *et al*., *J. Alloys Compd.*, vol. 859, 2021

[3] K. Martínez *et al., APL Mater.*, vol. 11, no. 10, 2023

#059	TUE	ENS	17:00 – 17:15	HS 9

Energy system models as a tool for the energy transition in Carinthia

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1.Task

The European Union and the Republic of Austria set binding targets and interim goals for energy and climate policy. On the one hand, this concerns the expansion of renewable energies, which must cover the final energy demand across all sectors. On the other hand, specific reduction targets for greenhouse gas emissions have also been set, leading to climate neutrality.

What will an energy system in Carinthia look like in 2040 that can cover the net energy demand while minimizing costs and meeting the political objectives and the technical potentials of renewable energies? What contribution do PtX and storage technologies make to such an energy system? For Austria and its federal states, it is already clear today that hydropower, photovoltaics and wind power will carry a great share of energy generation in the future. What areas must be available for the transition?

2. Approach

The energy system of Carinthia was modelled using the open energy system modelling framework *oemof*. Typical load and feed-in profiles, the existing potential of renewable energies and the sectoral energy demands were taken into account with a temporal resolution of 1 hour. The open-source licensed framework oemof is based on the Python programming language and provides various libraries for the configuration of energy systems. The model of the energy system implemented in oemof represents a linear problem. This is optimized by a solver either with regard to minimum costs or minimum CO2 emissions. The hereby used CBC solver is also licensed under the open-source licence.

3. Scenarios

The project considers two scenarios, each of which achieves Carinthia's energy and climate policy goals: Scenario A represents an innovative scenario characterized by a high willingness to use innovative technologies including hydrogen. In contrast, scenario B represents a technologically conservative scenario characterized by a slower rate of change and a trend towards all-electric solutions.

4. Results

The full paper presents transformation paths for scenarios A and B with the time horizons 2019-2030-2040. It discusses the need for action - for example for the spatial planning designation of areas for wind power and photovoltaics - and the scope for action - for example for the development of storage infrastructure.

#060	TUE	GEP	17:00 – 17:15	HS 10

Ground-based Observations at Lustbühel Radio Station (Graz)

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We report on the instrumental and research developments devoted to the study of Jovian and Solar decametric emissions at the Space Research Institute (SRI) in the period from 1985 to 2004. Helmut O. Rucker, the head of the Decametric Radio Team (DRT), emphasized on two aspects: the participation to the space missions (like Voyager and Cassini), and the deployment of new instruments (antenna and receivers) at Lustbühel Radio Station (Graz, Austria, 47°04'N, 15°26'E) in cooperation with European radio groups.

We highlight in our contribution on the ground-based investigations conducted at Lustbühel radio station where two Yagi antennas and a multi-channel radio receiver allowed the observations (1991-1994) of Jovian millisecond radio bursts. Those observations were performed first with the Nançay Decametric Array (Nançay, France) in 1991-1993, and later on with the Kharkov Radiotelescope (Kharkov, Ukraine) in 1995-2004. Also, we draw attention to the international cooperation allowed the development of a new generation of digital spectro-polarimeter tested in Nançay (France) and installed in Kharkov (Ukraine), and the establishment of a European Decametric Network. We review the main relevant scientific topics achieved towards a better comprehension of the magnetospheric physics of Jupiter, and the Solar-Terrestrial relationship.

#061	TUE	OGD 1	17:00 – 17:15	BA 9910

Birefringence in conventional TEM sample preparation

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Birefringent materials display thickness-dependent interference colors in transmission between two polarizers, a phenomenon published by Auguste Michel-Lévy at the end of the 19th century along with a color chart for various birefringence values. Polarized light passing through birefringent crystals splits into two components based on their refractive indices n_o and n_e, resulting in an optical path difference called retardation. Recombining both components with an analyzer leads to annihilation of specific wavelengths through destructive interference, revealing observable interference colors.

Our study leverages this phenomenon to optimize mechanical thinning in conventional sample preparation for transmission electron microscopy (TEM) [1]. We discuss our findings on dimpled and wedge-polished 4H-SiC/Al_2O_3 two-materials specimens. For materials with small birefringence, where interference colors vanish at larger thicknesses, we propose a complementary color chart for a parallel polarizer orientation, supplementing the Michel-Lévy chart valid for crossed polarizers. The thickness of the thinnest sample region can be estimated visually, with its color directly corresponding to the thickness on a color chart. The achieved accuracy of thickness monitoring, validated by scanning electron microscopy (SEM), significantly exceeds the measurement capabilities of built-in mechanical gauges in thinning instruments. Using simple geometrical models and complex RGB analysis the results can be further improved.

The proposed method streamlines mechanical thinning to low thicknesses, reducing the harmful ion-milling time to achieve electron transparency for TEM. Consequently, the sample amorphization can be reduced and the specimen quality improved. The method is not only useful for the presented substrate materials Al_2O_3 and SiC, but it can be applied to all other materials if birefringent materials serve as a thickness reference.

[1] A. Brozyniak *et al.*, Micron **177** (2024) 103580

#062	TUE	ENS	17:15 – 17:30	HS 9

Advanced Imaging & AI-based Analysis for Improved Energy Materials

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Improved energy materials are crucial for the transition towards sustainable energy systems. Artificial intelligence (AI) paves the way for accelerated design guidelines on the material and device level. Recently, machine learning algorithms have taken a big leap, and their utilization is far-reaching, e.g., for autonomous driving, natural language processing, or speech recognition devices. Furthermore, data driven approaches have also gained high interest, particularly to accelerate material development.

In this talk, we review our work, e.g. [1-3], on sophisticated characterization workflows employed in in the field of energy storage devices incorporating AI to derive enhanced material and device design guidelines. To get an in-depth knowledge of material degradation, we undertake highly sophisticated characterization investigations incorporating 2D-, 3D (tomography)-, and 4D (in operando: 3D and time)-imaging methods on diverse length scales. We provide information not only from the morphology but also from the chemistry as well as link different length scales, ranging from cm to nm. Furthermore, we demonstrate how sophisticated image data processing incorporating machine learning enhances the possibilities for an improved understanding of the structure-property relationship, an important ingredient for accelerated and improved material/device design. This AI-based approach allows for the rapid identification of critical material features and their correlation with performance, enabling the development of advanced energy materials with enhanced properties and durability. Moreover, it supports the design and optimization of energy materials, contributing to the advancement of energy storage and other critical energy technologies. This integration holds great promise for innovation and accelerating the transition towards a sustainable energy future.

[1] Multi-scale quantification and modeling of aged nanostructured silicon-based composite anodes | Communications Chemistry (nature.com)
[2] Impact of solid-electrolyte interphase reformation on capacity loss in silicon-based lithium-ion batteries | Communications Materials (nature.com)
[3] Analyzing microstructure relationships in porous copper using a multi-method machine learning-based approach | Communications (nature.com)

#063	TUE	GEP	17:15 – 17:30	HS 10

Österreich braucht keine Physiker...

Peter René Perez

Peter René Perez wird einen Auszug aus seiner Zeitzeugenrede zum Holocaustgedenken 2024 im spanischen Parlament in Madrid präsentieren, hier sein Lebenslauf in aller Kürze:

Geboren 1936 in Wien (Vater Bulgarier und sefardischer Jude, Mutter Wiener Katholikin), 1939 Flucht der Familie nach Frankreich, Internierung in verschiedenen Konzentrations- (Rivesaltes) und Arbeitslagern (Minen von La Caunette), Rückkehr 1948 nach Wien, Schüler im Lycée Français, Student der Angewandten Physik an der TU Wien, Angestellter der ÖMV (Datenverarbeitung), verheiratet und Vater zweier Kinder, Amateurboxer.

#064	WED	AMP 1	14:00 – 14:15	HF 9904

Gravitational redshift induces quantum interference

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General relativity and quantum mechanics are the two frameworks through which we understand Nature. To date, they have remained valid to great extent in their respective domains. Regardless of the myriad of attempts to find a unified theory that can describe all observable phenomena, consensus has not been reached and the quest for unification continues.

One avenue for investigating the overlap of general relativity and quantum mechanics that is less ambitious than theories of quantum gravity but can still provide potentially observable and measurable predictions is that of quantum field theory in curved spacetime viewed through the lens of quantum information. In recent years, a great deal of attention has been given to this approach, which has provided novel and intriguing insights into phenomena that can be also tested in the laboratory.

We present an investigation in the quantum nature of the gravitational redshift, seeking to understand which are the expected quantum dynamics that lead to such an effective classical observable effect. We discuss the relationship with the known regimes of applicability and show that more intriguing aspects are expected. We conclude discussing potential for detection in space-based experiments.

#065	WED	FAKT 3	14:00 – 14:15	BA 9911

Search for New Charmed Baryon States at the Belle II Experiment

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Charmed baryons are bound states of a heavy charm and two lights quarks (uds). While progress has been made in recent years, our knowledge of the charmed baryon is still sparse. E.g., by comparing with the known light baryon spectrum, at least 20 more states in the low-lying Sc spectrum should exist. By determining the charmed baryon spectrum and by comparing experimental findings to theoretical calculations will ultimately lead to a better understanding of numerical approaches to solve QCD in the bound state regime.

Using the data recorded with the Belle II detector at the e^+e^- collider SuperKEKB in Japan, we systematically explore the spectroscopy of single charmed baryons by reconstructing large samples of weakly decaying baryonic states ($\Lambda+_c$, Ξ^+_c and Ξ^0_c), combining them with photons, pions and kaons in the same event and searching the resulting $M(\Lambda^+_c X)$, $M(\Xi^+_c X)$ and $M(\Xi^0_c X)$ distributions for new excited baryonic states. In this contribution we present the current state of this research, which is focused on the selection and the measurement of the Λ_c and Ξ_c groundstates.

#066	WED	OGD 2	14:00 – 14:30	BA 9910

Momentum Microscopy of Organic-Metal Interfaces – Unravelling Mysteries of Charge Transfer

T. G. Boné[1], A. Windischbacher[1], F. Presel[1], P. Hurdax[1], L. Egger[1], M. S. Wagner[2], H. F. Bettinger[3], T. Jauk[4], F. Lackner[4], H. Peisert[2], T. Chassé[2], M. Schultze[4], P. Puschnig[1], M. G. Ramsey[1], G. Koller[1], M. Sterrer[1]

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Photoemission Orbital Tomography (POT) is an advanced form of angle-resolved photoemission spectroscopy, enabling the measurement of the complete photoelectron angular distribution in momentum space as a function of electron kinetic energy. This technique allows for an in-depth analysis of the electronic band structure of both organic and inorganic materials on metallic substrates, providing a comprehensive understanding of the sample's properties.

The NanoESCA Graz, a sophisticated photoemission microscope capable of imaging in both real and momentum space, was utilized to examine various innovative organic and inorganic surfaces using laboratory photon sources. This presentation demonstrates the efficacy of momentum microscopy and photoemission tomography in elucidating the electronic and geometric structure of surfaces, illustrated through experiments on heptacene/copper (110) oxide nanostructures.

Our combined experimental and computational findings reveal that when heptacene is aligned along the copper rows, both the lowest unoccupied molecular orbital (LUMO) and LUMO+1 become occupied. These findings, along with numerous others, offer fresh insights into charge transfer mechanisms and orbital configurations, unveiling previously unknown facets of this intriguing molecular system.

#067	WED	AMP 1	14:15 – 14:30	HF 9904

Weak values extraction from neutron interferograms

I. V. Masiello[1], A. Dvorak[1], H. Lemmel[1,2] and Y. Hasegawa[1,3]

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Since the first definition by Y. Aharonov, D. Albert, and L. Vaidman [1], weak values have gained an important role in the field of quantum physics. In particular, they have been shown to be strictly related to many fundamental concepts of quantum mechanics, such as: uncertainty relations [2], negative quasi-probability distributions [3], quantum paradoxes [4], and more [5]. Neutron interferometry has historically been a pillar in studying the foundations of quantum phenomena, and once more revealed itself to be a valuable tool for the study of weak values.

The 2 paths of an interferometer constitute a two-level quantum system: it is in all regards a qubit. Moreover, the established quantum nature of neutrons, which enter the interferometer one particle at a time, doesn't leave space to any other classical interpretation of the phenomena. Weak values of the path operators have been extracted by using an ancilla qubit, such as the spin of the neutron [6].

In our experiment we show that the full path weak value information (real and imaginary part) can be encoded in simple interferograms, without the need of auxiliary qubits. The experiment is realized using unpolarized neutrons traversing a triple Laue neutron interferometer with two phase shifters; one is used for the preparation and the other is for the manipulation of the state. The absence of polarization and spin analysis is a great advantage as it preserves a high neutron flux, significantly reducing the measurement time. The results clearly confirmed that it is possible to extract the real and imaginary part of the path weak values using interferograms.

[1] Aharonov, Yakir, David Z. Albert, and Lev Vaidman. "How the result of a measurement of a component of the spin of a spin-1/2 particle can turn out to be 100." Physical review letters 60.14 (1988): 1351.
[2] Hall, Michael JW. "Prior information: How to circumvent the standard joint-measurement uncertainty relation." Physical Review A 69.5 (2004): 052113.
[3] Dressel, Justin. "Weak values as interference phenomena." Physical Review A 91.3 (2015): 032116.
[4] Aharonov, Yakir, et al. "Revisiting Hardy's paradox: counterfactual statements, real measurements, entanglement and weak values." Physics Letters A 301.3-4 (2002): 130-138.
[5] Dressel, Justin, et al. "Colloquium: Understanding quantum weak values: Basics and applications." Reviews of Modern Physics 86.1 (2014): 307.
[6] Denkmayr, Tobias, et al. "Weak values from strong interactions in neutron interferometry." Physica B: Condensed Matter 551 (2018): 339-346.

#068	WED	FAKT 3	14:15 – 14:30	BA 9911

The CMS trigger system and its upgrade for HL-LHC

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The CMS experiment uses a two-level triggering system consisting of the Level-1, instrumented by custom-design hardware boards and delivering an output rate of the order of 100 kHz, and the High Level Trigger, a streamlined version of the offline reconstruction software running on a computer farm, which sends a rate of several kHz to permanent storage. This system has been evolving continuously since the startup of the LHC. While this system is still in use during the present LHC running period ("Run-3"), new features and algorithms are being developed to take care of higher data loads due to increasing luminosity and pileup but also of new experimental signatures to be investigated (in particular, displaced decay vertices stemming from relatively long-lived particles created in proton-proton collisions). Machine-learning techniques are being implemented in the trigger electronics and will occupy a more important place in the future. To avoid missing completely unexpected signatures from New Physics, studies are underway to employ anomaly detection using autoencoders.

A major upgrade of the triggering system will happen within the framework of the upgrade of the collider to the "High-Luminosity LHC (HL- LHC)", which will deliver a luminosity of $5 - 7.5 \times 10^{34}$ $cm^{-2}s^{-1}$, corresponding to 140–200 pileup events. An important difference from the present system will be the fact that after the upgrade, information from the silicon strip tracker will be available already for the Level-1 Trigger. This will allow CMS to use so-called "particle flow" objects, i.e. signals seen not only in one subdetector but put together from all available subdetectors, resulting in much sharper efficiency turn-on curves for trigger objects. Also, trigger rates will rise by a significant factor both at Level-1 (to 750 kHz) and at the High-Level Trigger, and the latency - the processing time available for arriving at the Level-1 trigger decision - will increase significantly, allowing for the use of more sophisticated algorithms at Level-1.

#069	WED	AMP 1	14:30 – 14:45	HF 9904

Testing infrared-induced decoherence in superconducting qubits

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Superconducting circuits are one of the main platforms for noisy intermediate-scale quantum computing. The quantum state encoded via excitations in the circuit must be protected from energy relaxation and dephasing. A prominent source of errors is the tunneling of unpaired excess electrons, referred to as quasiparticles, through the superconducting Josephson junction. We use charge-sensitive qubits as sensors and study the quasiparticle population in devices with niobium and tantalum base layers. We identify a) a significantly higher quasiparticle density in tantalum-based devices compared to niobium-based ones, and b) infrared as a major source of Cooper pair breaking, and study mitigation strategies for this background.

#070	WED	FAKT 3	14:30 – 14:45	BA 9911

The B0 meson lifetime measurement with the ATLAS experiment at CERN

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Recent results on the b hadron liftetimes using data taken with the ATLAS detector at the Large Hadron Collider are presented. They include measurements of the B0 lifetime from the decay to J/ψ K*, as well as of the B0 decay width Γd and the Γd/Γs width ratio, and of the effective lifetime in B0s decaying to a muon pair. Results are generally consistent with the Standard Model expectations.

#071	WED	OGD 2	14:30 – 14:45	BA 9910

Shape-Dependent Electrochemical Charge Injection and Transport in CdSe Nanocrystalline Thin Films

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Chalcogenide nanocrystals (NCs) are promising for affordable, energy-efficient solar cells, LEDs, and detectors. Hence understanding charge injection and transport in nanocrystaline thin film is crucial. The NC electronic band structure and surface properties influence charge injection efficiency. Electrochemistry combined with spectroscopy effectively identifies electronic band structures and examines the optical properties of charged NCs. Studying charge transport in NC thin films is vital for both fundamental science and practical applications in device fabrication.

In this work, we prepared and investigated the electrochemical charge injection mechanism in CdSe nanocrystalline thin films. The goal was to use spectro-electrochemistry (SEC), a combination of electrochemistry and spectroscopy, to understand the charge injection and transport mechanism in NC thin film. Boehme et al. [1] showed that beyond a specific size i.e., 3.7 nm of spherical CdSe quantum dots (QDs), charge injection is not possible in thin film configuration, whereas Arun et al. [2] showed charge injectionin 3.2 nm QDs in liquid phase. As the size of CdSe QD is reduced, the film becomes increasingly compact, which imposes constraints on electrochemical charge injection. These studies showed that the size and shape of the NC are essential parameters that determine the efficiency of charge injection into NC thin films. CdSe QDs are different from CdSe nanorods (NRs), not only in terms of energy band aliment [3], but also in terms the resulting thin film morphology, with NRs yielding less ordered films. However, so far, the information about the effect of morphology on the charge injection and transport in NC films has been limited. This work investigates the charge injection and transport mechanism in NC films assembled from NCs of various shapes and sizes. This investigation is complemented by in-situ spectroscopic characterization to better understand the kinetics and dynamics of optically generated charge carriers under an externally applied potential.

Acknowledgements.

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References.

1. Electrochemical Charging of CdSe Quantum Dot Films: Dependence on Void Size and Counterion Proximity. ACS Nano, 2013. 7(3): p. 2500-2508.
2. Spectroelectrochemistry of Colloidal CdSe Quantum Dots. Chemistry of Materials, 2021. 33(4): p. 1353-1362.
3. The Electronic Structure of Semiconductor Nanocrystals. Annual Review of Materials Science, 2000. 30(1): p. 475-521.

#072	WED	AMP 1	14:45 – 15:00	HF 9904

Universal dynamics in strongly interacting Bose gases far from equilibrium

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Universal dynamics of far from equilibrium system, within the last years, has seen an increasing interest in theoretical and experimental investigations. We report here the experimental study of strongly perturbed Bose gases and the observation of universal scaling behaviour during the relaxation of a non-equilibrium many-body system with strong interaction. Specifically, we present the self-similar scaling behaviour in momentum space in the infrared regime (particle transport) associated with the buildup of a Bose condensate. By varying the inter-particle interaction strength, the dependence of the duration of scaling evolution is observed. We find agreement of the universal scaling properties with the earlier rubidium experiment, signifying universality emergent across microscopically different experiments. We identify the suggested basin of attraction for the scaling evolution within both experiments via a generalized model of solitonic defects. Our results suggest a potential universal scaling law governing the far-from equilibrium relaxation and condensation of bosonic systems.

#073	WED	FAKT 3	14:45 – 15:00	BA 9911

Testing CPT symmetry with multi-strange baryons mass precision measurements using ALICE

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In any relativistic quantum field theory such as Quantum Chromodynamics or Electroweak theory, the interactions are invariant under the combined operation of Charge conjugation (C), Parity transformation (P) and Time reversal (T). One of the consequences of this (CPT) symmetry is that particles and their corresponding antiparticles must have exactly same mass. While the mass difference between proton and antiproton has been measured to a very high precision, the extension to (multi-)strange baryons domain still lacks precise measurements.

The ALICE detector is optimized to reconstruct decays of multi-strange baryons (Ξ and Ω). The collected data in pp at $\sqrt{s}$ = 13 TeV during the LHC Run 2 (almost two billion events), together with the particle identification capabilities of the ALICE detector, allow to measure the mass of the multi-strange hyperons and antihyperons with a very high precision. In this contribution, the mass differences between Ξ^- and Ξ^+, and between Ω^- and Ω^+ will be presented, sensibly improving the precision obtained by averaging the results from previous experiments.

#074	WED	OGD 2	14:45 – 15:00	BA 9910

2D Metal-organic frameworks on the (0001)-surface of the Topological Insulator Bi_2Se_3

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Topological insulators (TI) have fascinating electronic properties and thus have drawn much attention in the past 15 years. 3D TIs show strong spin-orbit splitting and time reversal symmetry (TRS) leading to topologically protected surface states with linear, Dirac-like dispersion. 2D heterostructures of TIs with other materials are highly interesting candidate structures for a variety of applications in new quantum devices and thus of considerable interest in quantum computing, optoelectronics or spintronics. Periodic arrays of ferromagnetically coupled transition metal (TM) atoms on the surface of a TI are predicted to spontaneously break TRS and induce a band gap opening at zero magnetic field (i.e., a quantum anomalous Hall effect, QAHE). A 2D metal organic framework (MOF) of spin-coupled TM atoms ordered by the right organic linkers could be such a candidate. [1]

Here, we investigate the self-assembly recipes of different cyano-group terminated linker molecules which successfully form 2D MOFs. One such candidate is dicyanoanthracene (DCA) [2, 3], for which we report the first-time realization of a 2D Fe-DCA MOF on the surface of Bi_2Se_3(0001). We apply a variety of surface science techniques (LEEM/LEED and STM) to investigate and characterize the formation of molecular islands from small to monolayer coverages, their chemical environment and electronic properties by photoemission spectroscopy and study the differences to the 2D MOF formation on metals, e.g. Ag and Au.

[1] Otrokov et al., Phys. Rev. B 92, pp. 165309(2015)
[2] D. Kumar et al., ACS nano 13, pp. 11882 (2019)
[3] L. Yan et al., Chem. Phys. Chem. 20, pp. 2297 (2019)

#075	WED	AMP 1	15:00 – 15:15	HF 9904

Coherent inflation in Bose-Einstein condensate

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In this work, we experimentally realized the coherent inflation by evolving a Bose-Einstein condensate of 87Rb on an inverted harmonic magnetic trap based on Atomchip. Within a short period, we obtained an expanded state with a coherence factor above 9. Furthermore, by optimally manipulating the magnetic potential with a designed time sequence, we largely restored the system back to the initial coherent state, demonstrating that the squeezing process can overcome the decoherence during the experiment time. The result validates the coherent inflation proposal based on inverted harmonic trap and can be applied in the levitated nanoparticle system, paving the way for weak force sensing and boosting the entangling rate of weakly interacting particles.

#076	WED	FAKT 3	15:00 – 15:15	BA 9911

The Fixed-Target Program at CERN's Secondary Beamlines and Test Beam Facilities

F. Stummer[1,2], E. Andersen[1], D. Banerjee[1], A. Baratto Roldan[1], J. Bernhard[1], M. Brugger[1], N. Charitonidis[1], L. A. Dyks[1], L. Gatignon[1,3], S. M. Gibson[2], A. Goillot[1], M. A. Jebramcik[1], F. Metzger[1], L. J. Nevay[1], E. G. Parozzi[1], B. Rae[1], S. Schuh-Erhard[1], L. Suette[1,4], M. Van Dijk[1], T. Zickler[1]

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CERN offers a diverse set of test beam facilities, providing a wide range of particle types over a large momentum spectrum. These secondary and tertiary beams are derived from the primary proton and ion beams of the PS and SPS accelerators, catering to fixed-target experiments and dedicated test beam areas. The beams available span from 0.1 GeV/c to 400 GeV/c, with a selectable flux ranging from several 100 to 10^9 particles per extraction.

This talk provides a comprehensive overview of all beamlines and available experimental areas. It also introduces the fixed-target experiments currently hosted in the beamlines, such as CLOUD, NA62, Amber, NA61/Shine, MuonE, NA64, the Neutrino Platform, and the newly approved dark matter search experiment SHiP.

#077	WED	OGD 2	15:00 – 15:15	BA 9910

Silver iodide surface structure and ice nucleation ability investigated by noncontact AFM

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Silver iodide (AgI) is used as a cloud seeding material due to its ability to nucleate ice efficiently, which is explained by the good lattice match between AgI and hexagonal ice. The basal (0001) cleavage plane of AgI deviates from the lattice of hexagonal ice by as little as 2.5%. However, AgI consists of stacked planes of positively charged Ag^+ alternating with negatively charged I^-. Cleaving a AgI crystal along the (0001) plane thus exposes Ag^+ and I^- terminated surfaces. Both terminations are polar and inherently unstable.

We present atomically resolved noncontact atomic force microscopy (NC-AFM) images that show how AgI(0001) surfaces compensate for this non-zero electric dipole perpendicular to the surface. Both Ag and I terminated surfaces form reconstructions, whose structure affects their ice nucleating abilities. NC-AFM images of UHV cleaved surfaces exposed to water vapor reveal that ice forms an epitaxial layer only on the Ag terminated surface, whereas on the I termination ice forms three-dimensional clusters.

These atomic-level observations could enhance our understanding of ice formation processes in the atmosphere.

#078	WED	AMP 1	15:15 – 15:30	HF 9904

Classical shadows for multi-qudit systems

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The classical shadows formalism introduced by Huang, Kueng and Preskill enabled the efficient prediction of numerous physical quantities of complex, large-scale quantum systems without requiring a full physical description. It comes with rigorous performance guarantees, ensuring its reliability and effectiveness. We extend the classical shadow formalism to n-qudit systems utilizing MUBs and SIC POVMs. We provide rigorous performance guarantees for estimating expectation values, quantum state fidelities, and purities, and trace inner products between two quantum states. Furthermore, we develop a new approach to estimating trace inner products and show the quadratically improved sample complexity. With this, we generalize a seminal result by Brydges et al. on estimating entanglement entropies via randomized measurements. We complement our theoretical findings with empirical studies highlighting that the actual protocols need fewer samples than theoretically anticipated.

#079	WED	OGD 2	15:15 – 15:30	BA 9910

Methanol and water compete for the same adsorption sites on $In_2O_3(111)$

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Indium oxide, a transparent conductive oxide, has been discovered to be a highly selective catalyst for methanol synthesis by CO_2 hydrogenation. The large surface unit cell of $In_2O_3(111)$ exhibits a variety of Lewis acid and base sites for methanol and water adsorption. We compare the adsorption of both molecules under UHV conditions by employing AFM, STM, XPS, and TPD, together with DFT calculations. For medium coverages up to 9 molecules per surface unit cell we find a similar behavior: Initially, at room temperature, both molecules dissociate and protonate the most reactive O sites of the unit cell. When both molecules are dosed consecutively, methanol readily replaces water, while water is less efficient to substitute methanol. Below 300 K, both methanol and water adsorb molecularly in less-favored regions of the unit cell, still occupying the same sites and thus forming the same structural motifs. However, at coverages beyond 9 molecules per unit cell significant difference are found due to the ability of water to form and receive two hydrogen bonds instead of only one in the case of methanol.

#080	WED	AMP 2	16:00 – 16:15	HF 9904

Low Energy Electron Interactions with Thiazole and 2-Bromo-5-Nitrothiazole

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In the modern treatment of tumors, one important problem is that a characteristic of solid tumors is the presence of areas of low oxygen content (hypoxia). Hypoxic cells often promote tumor metastasis and exhibit resistance to radiotherapy and chemotherapy. Radiation therapy uses high-energy radiation to bombard tumor cells. In this case the ionizing radiation leads to the release of a large amounts of secondary electrons, about $5*10^4$ per MeV deposited primary energy. These electrons possessing initial kinetic energies between 9-10 eV undergoes subsequent collisions with molecules present in the cells. This effect may be exploited for the utilization of radiosensitizer drugs, which should produce cytotoxic substances to increase the effect of the high-energy irradiation.

Here we studied the electron attachment induced fragmentation of thiazole and its derivative 2-bromo-5-nitrothiazole, which may represent a potential radiosensitizer. The experimental setup is a crossed-electron-molecule beams setup, including gas inlet system, hemispherical electron monochromator, quadrupole mass analyser and channel electron multiplier detector. The experiment was supported by quantum chemistry calculate. We report that thiazole and 2-bromo-5-nitrothiazole are efficiently decomposed by low-energy electrons with kinetic energies from 0 to 14 eV via single or multiple bond-cleavages. This behavior is beneficial to our understanding of the physicochemical properties of thiazole and 2-bromo-5-nitrothiazole, which is very important for the synthesis of related drugs and the potential application of radiosensitizers.

#081	WED	MBU	16:00 – 16:20	BA 9911

Structure-Mechanics Relationships of Heterodimeric Coiled Coils

Z. Atris[1], A.-M. Tsirigoni[1], M. Goktas[1], P. López García[1], R. J. Wilson[1,2], A. Valleriani[3], A. Vila Verde[4], K. G. Blank[1,2]

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Coiled coil (CC) structural motifs are found in a diverse array of different proteins. Consisting of self-assembled α-helices that create helical superstructures, they serve as key elements of cytoskeletal and extracellular matrix proteins. Despite their widespread occurrence as mechanical building blocks, the fundamental structural factors governing their molecular mechanical properties have remained largely elusive. We are applying AFM-based single molecule force spectroscopy and steered molecular dynamics simulations to determine the structure-to-mechanics relationship of *de novo* designed, synthetic CCs. When comparing heterodimeric CCs of varying length and sequence [1-4], our findings reveal that higher thermodynamic and kinetic stability does not always correlate with higher rupture forces within the range of AFM-accessible loading rates [4]. We further observe that a single sequence can exhibit diverse mechanical stabilities under different loading geometries. This knowledge is now utilized for the development of a library of CC-based mechanoresponsive hydrogel crosslinks for tissue engineering applications.

[1] M. Goktas, C. Luo, R. M. A. Sullan, A. E. Bergues-Pupo, R. Lipowsky, A. Vila Verde, K. G. Blank (2018) Molecular Mechanics of Coiled Coils Loaded in the Shear Geometry. Chem. Sci. 9:4610

[2] P. López-García, M. Goktas, A. E. Bergues-Pupo, B. Koksch, D. Varón Silva, K. G. Blank (2019) Structural Determinants of Coiled Coil Mechanics. Phys. Chem. Chem. Phys. 21:9145

[3] P. López-García, A. D. de Araujo, A. E. Bergues-Pupo, I. Tunn, D. P. Fairlie, K. G. Blank (2021) Fortified Coiled Coils: Enhancing Mechanical Stability with Lactam or Metal Staples. Angew. Chem. Int. Ed. 60:232

[4] A.-M. Tsirigoni, M. Goktas, Z. Atris, A. Valleriani, A. Vila Verde, K. G. Blank (2023) Chain Sliding versus β-Sheet Formation upon Shearing α-Helical Coiled Coils. Macromol. Biosci. 23:2200563

#082	WED	OGD 3	16:00 – 16:30	BA 9910

Electronic structure of a Moiré Dislocation Network at the $SrTiO_3$-$(La,Sr)(Al,Ta)O_3$ Interface

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Oxide interfaces offer unique possibilities to design phases with novel physics due to polar discontinuities, strain, and confinement effects. It was recently shown that strain relaxation leads to a highly ordered Moiré dislocation lattice at the interface between a $SrTiO_3$ (STO) thin film and its $(LaAlO_3)_{0.3}(Sr_2TaAlO_6)_{0.7}$ (LSAT) substrate. The electronic structure and therefore application prospects of this dislocation network remain unexplored. Using a combination of experimental and theoretical approaches, we here propose an atomistic model for the local ionic and electronic structure of these dislocation cores. Our results reveal a complex defect chemistry around the dislocations due to inherent oxygen deficiency coupled with cation interdiffusion that leads to reduced Ti^{3+} ions and consequently an increased electrical conductivity along the dislocation network.

#083	WED	AMP 2	16:15 – 16:30	HF 9904

Electron Collisions with Genistein

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Genistein (5,7-dihydroxy-3-(4-hydroxyphenyl) chromen-4-one), an isoflavone, mainly found in soybean and soy-derived products, has been well known for its anti-inflammatory, antioxidant and anti-proliferative properties. Recently, in radiobiological studies, genistein has shown its radiosensitisation potential for various types of cancers, however, the underlying molecular mechanism of this action has not been fully understood. Therefore, to better understand the behaviour of genistein, this study aims to investigative the interaction between genistein molecules and electrons – the most dominant secondary particles generated under irradiation. The experiment was performed with a crossed beam set-up incorporating a quadrupole mass analyser, which allows studying collision of electron beams and genistein molecules at isolated conditions. This approach first unveiled the fragmentation mechanism of genistein via electron ionisation at the electron energy of about 70 eV. Characteristic fragments resulting from Retro-Diels-Alder cleavage – a typical fragmentation pathway of naturally occurring compounds, dominate the electron ionisation spectrum. In the second set-up measurement, the intrinsic genistein properties were elucidated towards the low-energy electron attachment. Thereof, the molecular anion of genistein exhibits a remarkable stability, and only one fragment - dehydrogenated genistein anion has been observed.

#084	WED	MBU	16:20 – 16:40	BA 9911

Heterodimeric coiled coils as biological force sensors for early cell adhesion

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Coiled coil (CC) structural motifs are found in a diverse array of different proteins. Consisting of self-assembled α-helices that create helical superstructures, they serve as key elements of cytoskeletal and extracellular matrix proteins. Despite their widespread occurrence as mechanical building blocks, the fundamental structural factors governing their molecular mechanical properties have remained largely elusive. We are applying AFM-based single molecule force spectroscopy and steered molecular dynamics simulations to determine the structure-to-mechanics relationship of *de novo* designed, synthetic CCs. When comparing heterodimeric CCs of varying length and sequence [1-4], our findings reveal that higher thermodynamic and kinetic stability does not always correlate with higher rupture forces within the range of AFM-accessible loading rates [4]. We further observe that a single sequence can exhibit diverse mechanical stabilities under different loading geometries. This knowledge is now utilized for the development of a library of CC-based mechanoresponsive hydrogel crosslinks for tissue engineering applications.

[1] M. Goktas, C. Luo, R. M. A. Sullan, A. E. Bergues-Pupo, R. Lipowsky, A. Vila Verde, K. G. Blank (2018) Molecular Mechanics of Coiled Coils Loaded in the Shear Geometry. Chem. Sci. 9:4610

[2] P. López-García, M. Goktas, A. E. Bergues-Pupo, B. Koksch, D. Varón Silva, K. G. Blank (2019) Structural Determinants of Coiled Coil Mechanics. Phys. Chem. Chem. Phys. 21:9145

[3] P. López-García, A. D. de Araujo, A. E. Bergues-Pupo, I. Tunn, D. P. Fairlie, K. G. Blank (2021) Fortified Coiled Coils: Enhancing Mechanical Stability with Lactam or Metal Staples. Angew. Chem. Int. Ed. 60:232

[4] A.-M. Tsirigoni, M. Goktas, Z. Atris, A. Valleriani, A. Vila Verde, K. G. Blank (2023) Chain Sliding versus β-Sheet Formation upon Shearing α-Helical Coiled Coils. Macromol. Biosci. 23:2200563

#085	WED	AMP 2	16:30 – 16:45	HF 9904

Fourier transform mid-infrared spectrometry with undetected photons and prospective applications

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Mid-infrared (mid-IR) spectroscopy is a well-established method for obtaining high-quality chemical information. Thus, it is frequently applied in many fields, such as material characterization and biomedical research.

In recent years, a novel measurement principle that relies on quantum interference, namely metrology with undetected photons, has emerged and its practical applicability has been demonstrated. The method is inherently interferometric and involves the use of non-classical light sources. A quantum Fourier-transform spectrometer based on this sensing concept is presented in this contribution.

A nonlinear ppKTP crystal is used to generate entangled photon pairs through two sequential spontaneous parametric down conversion (SPDC) processes triggered by a pump laser (660 nm). Since the wavelengths of the idler and signal photons (in the case of non-degenerate SPDC) are spectrally widely separated by design (mid-IR, 4000 nm range; near-IR, 800 nm range), the technically well-developed Si-technology can be harnessed for IR metrology. Thus, high-sensitivity and high-resolution detectors can be used to perform routine mid-IR spectrometry. The two SPDC sources are coherent and interfere since the photon paths are indistinguishable (no absorption or scattering between the first and second SPDC process). The interference pattern breaks down when a correlated mid-IR photon is scattered or absorbed. This makes the technique of great interest for different application scenarios in mid-IR spectroscopy. Recent results are presented and discussed in this contribution.

References:

[1] A. Hochrainer et al., "Quantum indistinguishability by path identity and with undetected photons," Rev. Mod. Phys. 94, 025007 (2022).

[2] G. B. Lemos et al., "Quantum imaging and metrology with undetected photons: tutorial," J. Opt. Soc. Am. B 39, 2200-2228 (2022)

#086	WED	OGD 3	16:30 – 16:45	BA 9910

Probing Nanometer Features Beyond Topography: SPM as the Swiss Army Knife of Microscopy

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From field effect transistors and printable solar cells to 2D materials as the key functional component of novel applications, high-tech applications are becoming smaller and smaller. With this progressive miniaturization, an ever-challenging demand rises to study local features beyond mere topography on a relevant length scale. Here, scanning probe microscopy is a well-established technique that allows one to probe a multitude of parameters using an nm-sized tip attached to a force sensitive cantilever. Such cantilevers can be equipped with different lock-in amplifiers, current amplifiers, or resonant circuits to measure features like the local conductance, work function or mechanical properties like the adhesion and stiffness on a nm level.

In this talk, we showcase different examples of 2D materials and 2D heterostructures that were systematically investigated with different SPM-based techniques to provide a correlative set of measurements and thus provides a more comprehensive insight into the sample.

Namely, we present how Kelvin Probe Force Microscopy can be used to investigate the work function and charge accumulation locally, whereas conductive atomic force microscopy measures the conductance on a nm scale.

We outline, how such electronic properties can be correlated with nanomechanical features.

#087	WED	MBU	16:40 – 17:00	BA 9911

Bioinspired directional liquid transport

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This contribution deals with the design, fabrication, and functional principle of bioinspired microfluidic diodes capable of directional liquid transport. The devices are passive, i.e., there is no need for external energy input. They are capable of unidirectional water transport even against gravity. Backflow of liquid is prevented by the capillary forces in asymmetric capillary channels bioinspired by natural role models such as the integument of the Texas horned lizard (*Phrynosoma cornutum*) and the spermatheca of the rat flea (*Xenopsylla cheopis*). A key in these microfluidic systems is the specific geometry of the capillary channels and the contact angle of the test liquid on the substrate. Using the Young-Laplace equation, local liquid transport is described theoretically, which enables model-guided design. Rigid and stretchable proofs-of-concept were fabricated by means of laser ablation of poly(methylmethacrylate) (PMMA) plates using a CO_2 laser or by casting silicone into laser-engraved PMMA masters. PMMA is a low-cost technical polymer commonly used in disposable microfluidics. The topography of the fabricated 3D structures was analyzed by optical coherence tomography (OCT). Using optical flow analysis, fluid transport properties such as distance, velocity, wetted area, and flow asymmetry were analyzed. All tested devices showed directional liquid transport with velocities in the range of mm/s in the forward direction while preventing backflow. In the future, bioinspired directional liquid transport might be applied in biomedical microfluidics, labs-on-a-chip, micro-analysis devices, filtration, lubrication, cooling of electronics, and e-ink displays.

#088	WED	AMP 2	16:45 – 17:00	HF 9904

Vibrationally Induced Molecular Magnetism

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The first experimental observations and theoretical explanations of rotational and vibrational magnetism in molecules were made over 50 years ago, primarily during the peak of microwave spectroscopy research. Despite this, a comprehensive theoretical framework for this phenomenon is still lacking. In this talk, various models and approaches will be discussed, and their validity will be evaluated using selected molecules.

Given the recent interest in 'molecular magnets,' particularly those involving transition-metal complexes, we focus on metal phthalocyanines as our molecular platform, a versatile class of aromatic, planar, macrocyclic molecules with a chelated central metal ion. When twofold degenerate molecular vibrations are excited with a relative phase shift of $\pi/2$ between the two modes, it induces a rotational movement in each individual nucleus. This generates a total vibrational magnetic moment of the molecule, as well as intramolecular magnetic fields. These intramolecular magnetic fields may be observed as a vibrationally induced chemical shift.

While rotational and vibrational magnetism has been studied experimentally in form of g-factor measurements, an in-depth understanding of the theoretical foundation and the means to obtain reasonable theoretical predictions remain elusive. In our ongoing work, we derive relevant coupling parameters theoretically and perform ab initio calculations to obtain quantitative predictions for localized, vibrationally induced molecular magnetic fields.

#089	WED	OGD 3	16:45 – 17:00	BA 9910

Charge Exchange of Highly Charged Ions in 2D Materials

A. Niggas[1], F. Vukovic[1], F. Aumayr[1] and R. A. Wilhelm[1]

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Highly charged ions (HCIs) carry large amounts of potential energy, e.g., ~40keV for a Xe^{40+} ion, which results from the sum of binding energies of all removed electrons. Transmission experiments with 2D materials revealed that one layer of material can already be enough for complete neutralisation and deposition of this potential energy. The driving force behind this ultrafast deexcitation is the interatomic Coulombic decay (ICD), a distance-dependent Auger process, which is highly efficient at the small interatomic separations occurring during HCI-surface transmission [1].

Here we present a study of the neutralisation dynamics of HCIs in single-, bi-, and trilayer graphene samples by analysing the charge state of the ion after transmission for various kinetic energies and charge states. The results indicate that the neutralisation depends solely on the interaction time the ions spend in close proximity to the material layers [2]. Together with a simulation package modelling the HCI deexcitation via ICD [3], we establish a conceptual framework of ion deexcitation close to target atoms. As a conclusion, we apply this established knowledge to study amorphous organic nanosheets, which are challenging to characterise with traditional experimental techniques [4].

[1] R.A. Wilhelm *et al. Phys. Rev. Lett.* **119** 103401 (2017)
[2] A. Niggas *et al. Commun. Phys.* **4** 180 (2021)
[3] R.A. Wilhelm and P.L. Grande *Commun. Phys.* **2** 89 (2019)
[4] R.A. Wilhelm *et al. J. Phys. Conf. Ser.* **1412** 062010 (2020)

#090	WED	AMP 2	17:00 – 17:15	HF 9904

Selective Addressing of Nuclear Spins Through Pulsed Laser Excitation

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Nuclear electric resonance spectroscopy is experiencing a revival as a promising technique for quantum technologies using nuclear spins. This method utilizes electric fields to access nuclear spin states in contrast to commonly used magnetic fields. Electric control is enabled through the coupling of the quadrupole moment of a non-spherical nucleus and the electric field gradient generated by its surrounding. By conducting a thorough analysis of this coupling mechanism, we explore the feasibility of controlling nuclear spins in atoms and molecules using nuclear quadrupole interaction from first principles. We present a comprehensive, time-dependent framework and derive effective spin Hamiltonians, that include and reflect on commonly used approximations.

Using this approach, we introduce a completely new technique termed 'optical' nuclear electric resonance or 'ONER'. This protocol exploits time-modulated optical excitations via UV/visible light, for example realized by pulsed lasers, to manipulate the electric field gradient at the position of a given nucleus by periodic changes of the surrounding electron density. The concept is theoretically investigated for atomic and molecular benchmark systems, ranging from trapped atoms to medium-sized molecular structures. Our studies suggest that it might be possible to shift complicated spin manipulation tasks in atomic, molecular or solid-state systems into the time domain by time-modulated laser signals. Bringing optical excitation into play, the entire field of optoelectronics and nanophotonics might enter the quest for viable quantum technologies based on nuclear spin processes.

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#091	WED	OGD 3	17:00 – 17:15	BA 9910

Investigating 2D Layered Materials with Helium Atom Scattering

Surface structure and dynamics of layered 2D materials: InBi and InSe

V. Schwab[1], N. J. Hourigan[1], P. Seiler[1], B. Liu[2], M. Lin[2], A. Tamtögl[1]

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The field of layered 2D materials has become a vibrant topic of research due to their peculiar physical properties which can be adapted for future device applications. In my talk I will present measurements of the surface structure and dynamics of the 2D layered materials Indium-Bismuth (InBi) and Indium-Selenide (InSe). We employ Helium Atom Scattering (HAS) which has been demonstrated to be a sensitive probe for structure determinations and the surface phonon dispersion, in particular in the low-energy region [1].

Up to now, both materials have been predominantly investigated with first principle calculations. Monolayer InBi, has been predicted to exhibit ferroelasticity[2] and an extremely large magnetoresistance was measured in bulk InBi [3]. InSe on the other hand is a layered semiconductor which has been suggested as a possible alternative to silicon as active material in field-effect transistors with a first implementation in prototype studies [4,5].

Following the surface structure determination of InBi, we present the first measurements of acoustic surface phonons on InBi [5] and the dispersion is further compared with first principle calculations. For InSe, we illustrate based on diffraction measurements that the freshly cleaved surface undergoes a phase transition to In_2Se_3 after annealing at 380 K, likely to be related with increased Se diffusion and segregation in the surface region. Our experimental findings are further supported with quantum mechanical scattering calculations in order to determine the surface electronic corrugation of the layered materials InBi and InSe [6] and I will show that while InSe is very flexible with a weak interlayer bonding, InBi exhibits a much stronger bonding between the layers.

References

[1] A. Tamtögl *et al.*, *Nanoscale*, **10**, 14627 (2018)
[2] X. Ding *et al.*, *ACS Nano ,* **16**, 21546 (2022)
[3] K. Okawa *et al.*, Phys. Rev. Materials **2**, 124201 (2018)
[4] W.Wan *et al.*, *J. Phys.: Condens. Matter*, **35**, 133001 (2023)
[5] Ji. Jiang *et al.*, *Nature* **616**, 470–475 (2023)
[6] A. Tamtögl *et al.*, *Phys. Chem. Chem. Phys.*, **23**, 7637 (2021).

#092	WED	OGD 3	17:15 – 17:30	BA 9910

Investigating magnetic ordering in naturally occurring and artificially modified iron-rich phyllosilicates

M. Z. Khan[1]*, N. Klingner[2], G. Hlawacek[2], U. Kentsch[2], A. Ney[3], J. G. Raith[4], O. E. Peil[5], D. Knez[6], C. Teichert[1] and A. Matković[1]*

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The modulation of intrinsic 2D ferromagnetism has garnered significant attention and shown a great potential for spintronics. Although many two-dimensional (2D) van der Waals materials have been reported to exhibit intrinsic magnetism, there are still challenges when it comes to ambient stability, which is a crucial barrier for their integration into device application. We propose to overcome this by exploiting naturally occurring iron-rich phyllosilicates. Phyllosilicates offer a unique opportunity to explore complex air-stable layered systems with high concentration of magnetic ions. These naturally occurring layered materials are inherently magnetic and are wide band gap insulators (i.e. 5-6 eV). These minerals integrate local moment baring ions of iron via magnesium/aluminium substitution in their octahedral sites. Self-inherent capping by silicate/aluminate tetrahedral groups enables air stability of monolayers. Their structure and iron oxidation states are determined via Raman and X-ray spectroscopies. Superconducting quantum interference device magnetometry measurements are performed to examine the long range magnetic ordering. In-field magnetic force microscopy in the presence of externally applied magnetic field on exfoliated flakes confirms that the paramagnetic response at room temperature persists down to monolayers. We demonstrate correlations between the iron concentration, layer structure, iron oxidation states, and their magnetic response, indicating a path to design materials with higher critical temperatures via oxidation state engineering. Furthermore, we also demonstrate a scalable approach to control and tune the concentration of magnetic species via ion implantation into pure phyllosilicates crystals. Controlling the amount of implanted magnetic ions, choosing the dopant species or even alloying in the phyllosilicate matrix will open the pathways to engineer the 2D magnetic insulators with high critical ordering temperature.

#093	THU	AKCP	14:00 – 14:15	BA 9910

Innovative, geschlechtergerechte Physiklehre an Hochschulen

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In Physikvorlesungen und Physiklehrbüchern wird physikalisches Fachwissen vermittelt und zum Teil an Experimenten demonstriert. Darüber hinaus werden den Lernenden aber gleichzeitig meist nicht explizit ausgesprochen und oft sogar unbewusst zahlreiche Erzählungen über Physik vermittelt. Diese Narrationen handeln davon, wer von den Interessierten für ein Physikstudium geeignet ist und wer nicht, wer die Helden des Feldes sind, die aus ihrem genialen Geist die heutige Physik entwickelt haben, welche Werte und Verhaltensweisen in der Physikcommunity „normal“ sind oder welche Eigenschaften es braucht, um sich erfolgreich an der Weiterentwicklung der Physik beteiligt zu können. Noch viel zu oft werden dabei ungebrochen die Erfolgsgeschichten „alter weißer Männer“ erzählt.

Mit einem kulturwissenschaftlich-ethnologischen Blick auf Physiklehre in Vorlesungen und Lehrbüchern, wie ihn z.B. die Geschlechterforschung zur Physik einnimmt, können diese „heimlichen“ Narrationen sichtbar und ihre Ausschlüsse damit hinterfragbar gemacht werden. In meinem Beitrag werden anhand von konkreten Forschungsbeispielen und eigener Lehrerfahrung einer Physikvorlesung im Grundstudium des Maschinenbaus einige dieser Narrationen über Physik präsentiert. Es werden Lösungen vorgestellt, wie Erzählungen über Physik vielfältiger gestaltet werden und Physiklehrende damit selbst zur Erhöhung der Attraktivität der Physik für eine breitere Zielgruppe beitragen können. Dabei wird auch ein Beispiel thematisiert, wie Digitalisierung zu einem Verfestigen oder Aufbrechen traditioneller Vorstellungen einer „männlichen, weißen Physik“ beiträgt bzw. sinnvoll genutzt werden kann.

#094	THU	COND 3	14:00 – 14:30	HS 9

Integrated Plasmonics for Mid-infrared Photonic Circuits

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Photonics has revolutionized global communication and data processing, transforming connectivity in the digital age. Photonic integrated circuits (PICs) have further advanced this field by enabling compact and cost-effective optical systems and sensors. While visible and near-infrared photonics have been extensively explored, resulting in mature commercial products, mid-infrared (mid-IR) photonics has only recently garnered attention. The recent development of intersubband devices has led to the creation of highly efficient emitters and detectors, unlocking their potential in diverse fields such as free-space optical communication, medical diagnostics, defense, and security. Despite these advantages, the development of mid-IR PICs faces challenges due to the limited availability of suitable materials and efficient integration strategies. Plasmonics offers a promising solution to these challenges by utilizing metallic structures combined with insulating materials to create dielectric-loaded surface plasmon polariton waveguides (DLSPPWs), capable of effectively guiding and manipulating light on the chip surface. This work focuses on overcoming these obstacles and advancing fully integrated mid-IR PICs using DLSPPWs. Specifically, we study the properties of germanium (Ge) and polyethylene (PE) ridges deposited on top of gold layers and investigate their potential for mid-IR sensing and on-chip mode guiding. PE, known for its transparency and low refractive index, demonstrates effective performance in the long-wave infrared (LWIR, 8-12 µm) spectrum, balancing propagation length and mode confinement. Thin Ge slabs exhibit properties ideal for broadband propagation (2-14 µm) with substantial tunability, making them well-suited for sensing applications. Furthermore, as a proof-of-concept, we explore the potential of the aforementioned Ge-based waveguide sensors tailored for mid-IR applications. Finally, integrating low-loss Ge waveguides with on-chip micro-mirrors enables the realization of compact, versatile, monolithic PICs. As an exemplary application, an LWIR heterodyne detector operable at room temperature shows the potential of these advancements. The significant progress in developing highly integrated, monolithic mid-IR PICs demonstrated in this work complements the ongoing advancements in quantum cascade intersubband devices, paving the way for advanced communication and sensing applications.

Major Contributions:

Marschick, G. [1], Arigliani, E. [1], Dabrowska, A. [2], Disnan, D. [3], Sistani, M. [1], Nazzari, D. [1], A., Detz, H. [1], Schmid, U. [3], Lendl, B. [2], Schwarz, B. [1], Andrews, A.M. [1], Strasser, G. [1], Hinkov, B.[1]

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[…]

#095	THU	PIN 1	14:00 – 14:30	HS 10

A career path as a physicist in industry (and what you can rely on from your education)

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My career path in industry has taken me from expert roles to leadership roles in teams of various sizes to my current position as Head of Research and Development at Swarovski. It has become clear to me that as a physicist, you are taught a tool set during your studies that helps you in every job along the way and in all situations.

At the beginning, in an expert role, you benefit from the specialist knowledge that you are taught in sufficient breadth and the fundamental thinking that the explanatory models of natural science shift and develop over time. Interestingly, the set of methods used in physics can be applied just as well in management positions - analytical thinking, using thought models to develop strategies or establish leadership, using mathematics and statistics, establishing processes and maintaining an overview in complicated situations. I will show this using individual stages of my career path.

#096	THU	AKCP	14:15 – 14:30	BA 9910

The invisible CV: career insights from a first-generation woman professor

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Women pursuing higher education and academic careers often face unique challenges, contributing to the "leaky pipeline" phenomenon [1]. While diversity surveys and reports frequently assess gender and ethnicity, they often overlook educational background, rendering it an invisible factor. This oversight is crucial, as first-generation academics encounter numerous challenges that add to other minority factors [2]. These include navigating unfamiliar academic environments, lacking role models, mentorship and support networks, dealing with imposter syndrome as well as managing financial constraints. In this presentation, I will share my experiences as a first-generation woman in interdisciplinary physics research. I will focus on (a) the absence of role models and encouragement, which led to (b) an unconventional career path, and (c) the ongoing struggle to bridge two very different worlds. Addressing these specific challenges from a broader perspective is essential to support and inspire first-generation students and to foster a diverse academic environment and an inclusive educational landscape. In Austria, only 12% of children from non-academic parents achieve a university degree, indicating that the promise of upward social mobility through education remains unfulfilled [3]. The academic sphere and society as a whole cannot afford to overlook the unique experiences, remarkable resilience, fresh perspectives and innovative insights that first-generation women and other first-generation academics bring to the table.

[1] J. C. Blickenstaff (2005) Women and science careers: leaky pipeline or gender filter?. Gender Educ. 17:369
[2] C. A. Bauer & V. Job (2024) Double disadvantage: Female first-generation-students think of themselves as least talented, contributing to disproportionate disadvantage. Learn. Instr. 90:101865
[3] S. Achleitner (2022) Bildungsreport - Ein Pay Gap kommt selten allein: Bildung, Gender und Einkommen in Österreich. Momentum Institut, Wien, Austria

#097	THU	AKCP	14:30 – 14:45	BA 9910

Der Arbeitskreis Chancengleichheit: Seine Bedeutung und die Projekte seit 25 Jahren

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Der Arbeitskreis Chancengleichheit AKC in der Deutschen Physikalischen Gesellschaft DPG besteht seit über 25 Jahren und hat das Ziel, die Rahmenbedingungen für Physikerinnen zu verbessern. Wir haben dazu Umfragen bzw. Studien initiiert, um die unterschiedliche Situation von Physikerinnen im Vergleich zu Physikern mit Zahlen belegen zu können. Zahlen des Statistischen Bundesamt werten wir aus, um Veränderungen zu erkennen und unsere Arbeit zielgerichtet durchführen zu können. Wir unterstützen Tagungen, der Deutschen Physikerinnentagung DPT, die Frühjahrstagungen der DPG, International Conference on Women in Physics ICWIP mit Vorträgen zum Thema Chancengleichheit und mit Zahlen zur aktuellen Situation. Workshops für Physikerinnen, die "Physikerin der Woche" und das Projekt "Faszination Wissenschaft!", um dem Nachwuchs Vorbilder präsentieren zu können. Da die Leistungen von Physikerinnen nicht genug durch Preise gewürdigt wurden, ist der Hertha Sponer-Preis, auf unsere Initiative geschaffen worden. Es gibt noch genug zu tun. Die Zusammenarbeit mit anderen Physikalischen Gesellschaften unterstützt unsere Arbeit. Darüber werde ich berichten.

#098	THU	COND 3	14:30 – 14:45	HS 9

STED-inspired two-photon lithography of EDOT nanostructures

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In the rapidly evolving field of nanoelectronics, poly(3,4-ethylenedioxythiophene) (PEDOT) stands out among conductive polymers for its high electrical conductivity and thermal stability [1]. However, traditional PEDOT production methods, such as chemical and electrochemical polymerization, often lack the spatial precision needed for advanced nanoelectronic applications.

Multiphoton polymerization (MPP) excels in creating 3D structures in one step, avoiding the traditional layer-by-layer approach [2]. Controlling two-photon absorption with low-energy near-infrared femtosecond laser pulses prevents damage to sensitive materials like organic semiconductors or biomaterials. Although limited by diffraction, super-resolution methods like stimulated emission depletion (STED) enhance resolution by confining polymerization to the laser's point spread function (PSF) center [3]. For instance, transient absorption depletion (TAD) lithography, inspired by STED, uses long-living transient states to stop polymerization, preventing radical formation or electron transfer from them and refining polymerization to smaller volumes [4].

In our current study, we implemented these sub-diffraction lithography principles to the oxidative polymerization of EDOT. We discovered that 7-diethylamino-3-thenoylcoumarin (DETC), typically used as a photoinitiator for STED-inspired radical photopolymerization, can also serve as a photosensitizer for EDOT oxidative polymerization. Additionally, using DETC in TAD-lithography enabled us to produce sub-100 nm PEDOT nanostructures.

References

[1] Alamer, F., et al. "Review on PEDOT: PSS-based conductive fabric." ACS Omega, 7.40 (2022): 35371-35386.

[2] Maruo, S.; Nakamura, O.; Kawata, S. "3D microfabrication with two-photon-absorbed photopolymerization." Optics Letters, 22 (1997): 132-134.

[3] Fischer, J.; Wegener, M. "3D direct laser writing inspired by STED microscopy." Optical Materials Express, 1.4 (2011): 614-624.

[4] Gvindzhiliia, G., et al. "Low-Fluorescence Starter for Optical 3D Lithography of Sub-40 nm Structures." ACS Applied Optical Materials, 1.5 (2023): 945-951

#099	THU	PIN 1	14:30 – 15:00	HS 10

Austrian Primary Standards for Humidity/Dew Point, Air Velocity and the Amount of Substance frac<on CO_2 and their Traceability to the SI Base Units

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At the 26th General Conference on Weights and Measures (CGPM) in the year 2018, the revision of the International System of Units (the SI) was agreed and the base units were presented in a new format. The new definition changed the physical concept of the definition of the kilogram, the ampere, the kelvin and the mole, namely it uses the constants of nature instead of referring to an artifact.

The Designated Institute (DI) of E+E Elektronik GesmbH has developed and is operating three Austrian Primary Standards, namely for Humidity/Dew Point, for Air Velocity and for the amount of substance fraction carbon dioxide. These standards are directly traceable to the International System of Units and deliver therefore international comparable and accepted measurement results. These standards are regularly checked through key comparisons that are organized by the BIPM (Bureau International des Poids and Messures) which is the representative of the Worldwide Society of Metrology. The Designated Institute disseminates the measurement quantities together with a complete measurement uncertainty budget to the accredited calibration laboratories which in turn pass them on to the Industrie. The dissemination takes place with a certificate in which the deviation of the device unter test from the primary standard and the corresponding measurement uncertainties are depicted.

In this presentation the construction of Austrian Primary standards, their traceability to the International System of Units and the International Metrology System are described as well as my professional career until now. Remember that industrial collaboration and global production are only possible with an internationally consistent and recognized measurement system that actually dates back to the signed Meter Convention of 1875.

#100	THU	NESY	14:45 – 15:00	HS 9

3D microstructural analysis of novel scaffolds for bone tissue repair and regeneration

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The field of tissue engineering has shown great promise in its potential to address tissue-related defects and injuries. 3D structural and functional scaffolds to mimic natural tissues. A controlled mechanism has to be optimized. Tissues from animals and humans have complex hierarchical architectures at multiple length scales. Successful biomimicry required for the repair and regeneration of functional tissues requires a complete understanding of the 3D architectures. Microtomography using synchrotron X-rays is a powerful tool to visualize, analyze, and explore these structures three-dimensionally. This technique is non-destructive and no sample preparation is required. Our objectives are to investigate the 3D morphology and evaluate the microarchitecture of these porous biomaterials. Qualitative and quantitative studies are essential. Features like porosity, phases, and fibers will be investigated. This will help to optimize the controlled mechanism for suitable pore size and adequate mechanical strength. Thereby leading to the development of functional biomaterials that are affordable and reliable to be introduced into the healthcare sector.

[1] Sarfaraz, Sehrish, et al. Int. J. Polym. Mater. 72.15 (2023)
[2] Lee, Seunghun S., et al. Matter 5.9 (2022):
[3] Wang, Menglong, et al. Materials Highlights 1 (2020)
[4] Santonocito, Simona, et al. Exploration of Medicine 4.2 (2023)
[5] Vu, A. A., & Bose, S. RSC advances, 9(60), (2019).
[6] Petre, D. G., & Leeuwenburgh, S. C., Tissue Engineering Part B: Reviews, 28(1), (2022).

#101	THU	NESY	15:00 – 15:15	HS 9

Core/Shell/Shell Structure of Nanocrystals using Environmentally Benign Material Compositions

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Chemical synthesised colloidal nanocrystals (NCs) offer the opportunity for realising novel semiconducting materials with tailored functionalities, e.g. for creating quantum dots (QDs) for light emission [1]. Especially an inner core/shell structure of semiconducting NCs leads to an increased photoluminescence (PL) output, that means to a high quantum yield (QY) of the QDs [1, 2, 3]. We have revealed a relation between structure, shape and functionality by combining different scattering techniques at lab and synchrotron sources with microscopy techniques [2, 3]. In a study at the synchrotron ESRF, we have investigated CdSe/CdS core/shell NCs with different dimensions by recording anomalous scattering and diffraction (ASAXS/WAXS) patterns [2]. The knowledge gained on this environmentally not-friendly material system was applied now to the characterisation of a non-toxic material system, used for the fabrication of core/shell/shell QDs that reach a high quantum yield of ~91% [3]. The inner structure of the environmentally benign InP/ZnO/ZnS core/shell/shell QDs was investigated by lab based small angle x-ray scattering (SAXS) and XRD characterisations in Leoben, as well as synchrotron based SAXS at ELETTRA. The results show that spherical InP core and InP/ZnO core/ shell NCs turn into elliptical particles with the growth of the second ZnS shell [3]. Furthermore, due to the sub-nanometer resolution of SAXS we could follow the shell growth during synthesis in monolayer step accuracy. This allows to better understand the wet chemical synthesis of these core/shell/shell NCs and hence to optimize their PL-output.

[1] M. V. Kovalenko, et al., & W. Heiss, ACS Nano **9**, 1012–1057 (2015)
[2] L. Ludescher, et al., & R.T. Lechner, Front. Chem. **6**, 672 (2019)
[3] G.O. Eren, et al., & R.T. Lechner, S. Nizamoglu, ACS AMI **13** (2021)

#102	THU	PIN 1	15:00 – 15:30	HS 10

From Low Temperature Physics to Molecular Biology or How I learned to be a multi-disciplined multi-tasking physicist

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My name is Barbara Stadlober and I am a principal investigator at MATERIALS - the Institute for Sensors, Photonics and Manufacturing Technologies - of the JOANNEUM RESEARCH Forschungsgesellschaft mbH (JR). In the course of my career, I have already covered a broad spectrum from low-temperature physics to semiconductor technology, electronics and biomedical diagnostics. After finishing experimental physics at the Karl-Franzens University in Graz, I received my PhD from the Technical University in Munich-Garching for my work about electronic Raman scattering in high temperature superconductors. Although I loved working in basic research, I dreaded the somewhat nomadic existence of successive temporary postdoc positions and therefore decided to start as a reliability engineer in the technology development team of Siemens Halbleiter AG, later Infineon Technologies in Villach. But 6 years and two children later, research called again and so I joined JR in 2002 to set up a new research team for organic and printed electronics as well asscalable micro/nanopatterning techniques. Meanwhile the group is called “Hybrid Electronics and Patterning” and has about 30 scientists. We develop everything that can be integrated on a flexible substrate, be it organic thin-film transistors, printed ferroelectric sensors, nanogenerators, bionic and microoptical surfaces as well as microfluidic lab-on-a-foil chips for medical diagnostics and biosensing. This resulted in about 120 peer-reviewed publications, a reasonable number of patents, close collaboration with industry and participation in numerous (currently 16) European Research Projects from all three pillars of the Horizon Europe Program.

#103	THU	NESY	15:15 – 15:30	HS 9

Investigating ion dynamics in capacitive de-ionization using in-situ X-ray techniques

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Capacitive deionization (CDI) is an essential technique for water desalination or brackish water treatment. The basic principle relies on capturing ions from a feed water stream within an electrochemical flow-cell at electrical double layers (EDL) of charged nanoporous electrodes. In this study, X-ray transmission imaging (XRT), and small-angle X-ray scattering (SAXS) are employed to provide a detailed analysis of temporal and spatial variations of ion concentration along the flow path in the electrodes.

The experiments utilized commercial activated carbon electrodes (MSP20) with PTFE binder and CsCl and NaCl electrolytes at different concentrations and different flow rates. A custom designed electrode with a pattern of small punched holes or stripes in the two electrodes enabled the collection of X-ray data from both electrodes as well as the bulk electrolyte solution in the separator between the two electrodes separately.

Significant changes in ion concentration were observed between static and flow conditions, notably demonstrating enhanced counter-ion adsorption under flow conditions. Additionally, variations in ion concentration relative to the flow inlet position were observed and attributed to local concentration changes in the feed solution as ions were stored along the flow path in the electrodes.

#104	THU	COND 4	16:00 – 16:15	HS 9

Nanoscale electrical characterization of a multiphase intermetallic γ-TiAl alloy

M. Kratzer[1], M. Huszar[1], L. Tengg[2], T. Billovits[3], B. Kaufmann[3], P. Supancic[3], H. Clemens[2], S. Mayer[2], and M. C. Teichert[1]

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Novel light-weight high-temperature structural materials are crucial when high performance meets low-energy consumption. Possible candidates are intermetallic γ-TiAl-based alloys, which – in terms of weight – outperform conventional Ni based alloys. Besides their mechanical properties, like high specific strength and high creep resistance, also their electrical behavior is of significant importance. Otherwise a correct interpretation of electrical material testing techniques, like eddy current testing, is impossible. Here, local-probe techniques, like conductive atomic force microscopy (CAFM) and micro four-point probe (μ4PP) measurements, were used to directly determine the specific resistivity of the constituent phases of a technical sample made of a Ti-43.5Al-4Nb-1Mo-0.1B (at%) TNM γ-TiAl based alloy. The different phases turned out to have clearly different resistivity values varying over two orders of magnitude. CAFM and μ4PP results were in rather good agreement for the α_2 and γ phases with resistivity values of $\rho_{\alpha2,CAFM}$ =(1.0±0.7)×10^{-5} Ωm and $\rho_{\alpha2,4PP}$ = (3.4±3.5)×10^{-5} Ωm for the α_2- phase, and $\rho_{\gamma,CAFM}$ = (6.5±2.1)×10^{-6} Ωm and $\rho_{\gamma,4PP}$ = (3.1±2.0)×10^{-6} Ωm for the γ-phase. For the β_o phase, μ4PP measurements resulted in $\rho_{\beta o,4PP}$ = (1.0±1.7)×10^{-7} Ωm. In this case, CAFM values were deteriorated due to the formation of a contact barrier.

#105	THU	PIN 2	16:00 – 16:30	HS 10

„Curiosity as a Career Driver? – a practical example“

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Curiosity as a career driver? - a practical example.

Sound with its wave character is basically a physical phenomenon. Sound is essential, even indispensable, in our lives when we think of language and communication. However, sound also has undesirable side effects: Sound as noise, as unwanted sound - which adds perception to physics.

My current main field of activity is the strategic discussion of railway noise at ÖBB-Infrastruktur AG and the railway system. Where and how noise is generated, how it can be reduced, how it propagates and how all this is regulated by law. And just as sound does not only propagate in a straight line as a sound beam, careers do also not always follow a straight line either: they can be driven by coincidences, quasi interfering with other aspects of life, that were not initially realised or considered. As an example, my quasi ‘meandering’ professional career might provide inspiration to explore something like a ‘career’ - at least in retrospect - with the variety of topics in physics and characteristics such as openness, but especially curiosity.

Neugier als Motor von Karriere? – ein Praxisbeispiel.

Schall mit seinem Wellencharakter ist im Grunde ein physikalisches Phänomen. Schall ist wesentlich, ja unverzichtbar in unserem Leben, wenn man an die Sprache, die Kommunikation denkt. Schall hat aber auch unerwünschte Nebeneffekte: Schall als Lärm, als nichterwünschter Schall – womit die Physik um die Wahrnehmung erweitert wird.

Mein derzeitiges Haupt-Tätigkeitsfeld ist die strategische Auseinandersetzung mit Bahnlärm in der ÖBB-Infrastruktur AG bzw beim System Eisenbahn. Wo & wie entsteht Schall, wie kann dieser verringert werden, wie erfolgt die Ausbreitung, bis hin zu dem, wie all dies rechtlich geregelt wird. Und so wie sich Schall nicht nur geradlinig als Schallstrahl ausbreitet, so verlaufen Karrieren auch nicht immer geradlinig: sie können von Zufällen getrieben sein, quasi interferieren mit anderen, zunächst nicht ge- bzw bedachten Aspekten. Als ein Beispiel soll mein quasi ‚mäandernder‘ beruflicher Werdegang Anregung bieten, um mit der Themenvielfalt der Physik sowie Eigenschaften wie Offenheit, aber insbesondere Neugier so etwas wie eine ‚Karriere‘ – zumindest im Nachhinein – zu ergründen.

#106	THU	COND 4	16:15 – 16:30	HS 9

Quantum Fisher information in quantum critical $Ce_3Pd_{20}Si_6$

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Strange metal behavior is observed across many materials platforms; its understanding represents a key open problem in correlated quantum matter [1]. Common features beyond the "strange metal" linear-in-temperature electrical resistivity are the accumulation of entropy, a jump of the Fermi volume and the energy-over-temperature scaling in dynamical susceptibilities [2]. The heavy fermion compound $Ce_3Pd_{20}Si_6$ [3,4] is an ideal testbed not only to probe quantum criticality that goes beyond the Landau-Gizburg-Wilson paradigm through the evaluation of the fractional quantum critical exponent but also to investigate new theoretical predictions regarding multipartite entanglement [5]. We present the results of our recent inelastic neutron scattering investigation at a strange metal quantum critical point in $Ce_3Pd_{20}Si_6$, including the dynamical scaling, the quantum Fisher information density f_Q, and a comparison with quantum Monte Carlo simulations on a pertinent model [6].

[1] Checkelsky, J. G., Bernevig, B. A., Coleman, P., Si, Q. & Paschen, S. Flat bands, strange metals, and the Kondo effect, Nat. Rev. Mater. (2024). https://doi.org/10.1038/s41578-023-00644-z.
[2] Paschen, S. & Si, Q. Quantum phases driven by strong correlations, Nat. Rev. Phys. 3, 9–26 (2021).
[3] Martelli, V., Cai, A., Nica, E. M., Taupin, M., Prokofiev, A., Liu, C.-C., Lai, H.-H., Yu, R., Ingersent, K., Küchler, R., Strydom, A. M., Geiger, D., Haenel, J., Larrea, J., Si, Q. & Paschen, S. Sequential localization of a complex electron fluid, Proc. Natl. Acad. Sci. U.S.A. 116, 17701 (2019).
[4] Custers, J., Lorenzer, K., Müller, M., Prokofiev, A., Sidorenko, A., Winkler, H., Strydom, A. M., Shimura, Y., Sakakibara, T., Yu, R., Si, Q. & Paschen, S. Destruction of the Kondo effect in the cubic heavy-fermion compound Ce3Pd20Si6, Nat. Mater. 11, 189 (2012).
[5] Hauke, P., Heyl, M., Tagliacozzo, L. & Zoller, P. Measuring multipartite entanglement through dynamic susceptibilities, Nat. Phys. 12, 778–782 (2016).
[6] Mazza, F., Biswas, S., Yan, X., Prokofiev, A., Steffens, P., Si, Q., Assad, F. & Paschen, S. Quantum Fisher information in a strange metal, arXiv:2403.12779.

#107	THU	COND 4	16:30 – 16:45	HS 9

Hidden beneath microstructural constraints: Revealing the displacive nature of grain boundary migration using electron and atomic force microscopy

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It is accepted that thermally induced (i.e., curvature driven) grain boundary migration (GBM) occurs by diffusive jumps of atoms across the GB. The associated GB velocity is believed to be proportional to the product of GB mobility and the driving force, equal to GB curvature in case of thermally driven motion. Recent 4D analyses of microstructural evolution question this fundamental equation - no relationship between GBM velocity and GB curvature was found for polycrystals. This indicates that the true physical nature of GBM is not captured in current models.

Rather than by diffusive jumps, molecular dynamics simulations suggest that GBM may proceed in a militaristic manner by GB line defects, termed GB disconnections (GBDs). This defect consists of a step height, h, and a Burgers vector, $\boldsymbol{b}$. Upon migration of GBDs, the GB moves by multiples of the step height but this motion is associated by a shear in the direction of $\boldsymbol{b}$. This suggests that GBM is inherently coupled to a plastic displacement, not observed so far upon annealing treatments of polycrystalline materials as the constraint of the polycrystalline network would inhibit the potential shear displacement.

However, sufficiently sensitive surface measurements or the use of thin specimens could allow to detect this shear-coupled GBM. We thus used AFM topography imaging in tapping mode to measure - at the polished surface of a polycrystal - the out-of-plane motion of single GBs during its migration. By comparing a statistically relevant number of static and mobile GBs, the shear-coupled motion could be confirmed.

#108	THU	PIN 2	16:30 – 17:00	HS 10

The world of precision optics manufacturing – challenges and possibilities for physicists

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The fabrication of highly precise optics presents a broad spectrum of challenges. Achieving surfaces with a roughness within the angstrom scale and shape deviations in the nanometer range demands extensive manufacturing expertise alongside ongoing advancements in process engineering and measurement technology.

SwissOpticAG specializes in the manufacturing of precision optical components and optical systems. It covers the entire value chain, from cutting the raw glass block over high-end coatings to system engineering and integrating comprehensive optical systems.

Physicists at SwissOptic AG work across various departments. For example, they contribute to product development, designing specialized metrology systems, and improving manufacturing processes. This talk gives insides into the role of a laser technologist and the diverse opportunities available within the manufacturing technology team. Furthermore, it aims to outline other career paths for physicists in an optics manufacturing company.

#109	THU	COND 4	16:45 – 17:00	HS 9

Negative Longitudinal Magnetoresistance in the Dirac Semimetal $PtSe_2$ – Kondo Effect and Surface Spin Dynamics

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Transition-metal dichalcogenides (TMDs) support a plethora of exploitable features, such as the chiral magnetic effect (CME), type-II Dirac cones breaking the Lorentz invariance and topologically non-trivial surface states [1]. The TMD $PtSe_2$ is a top-contender for applications in the next generation of electronic, spintronic and photonic devices, offering topological characteristics combined with high electronic mobility, significant spin-orbit-coupling owing to Pt, and stability under ambient conditions.

In order to probe the electronic properties of $PtSe_2$, low-T/high-$\mu_0 H$ transport is carried out on exfoliated flakes. In particular, the origin of the detected negative longitudinal magnetoresistance (NLMR) is explored, which is crucial for the understanding of the emergence of type-II Dirac cones and of the previously reported CME [2]. The source of the NLMR is identified in the Kondo effect and a transport model is introduced, which captures, how the Kondo effect sets in at $T \lesssim 15$ K and how the polarization of the impurity spins reduces the Kondo scattering upon application of an external magnetic field. The model also describes the anisotropic orbital magnetoresistance. By applying density functional theory in conjunction with different flake thicknesses, the impurity spin sites are identified as Pt-vacancies contributing an uncompensated spin density at the sample surface. The results point at both the sample thickness and the Pt-vacancy concentration as tuning parameters for the control of the emergent 2-dimensional spin density and of the interplay between the Kondo effect and orbital magnetoresistance in the system.

[1] N. P. Armitage, E. J. Mele, and A. Vishwanath (2018) “Weyl and Dirac semimetals in three-dimensional solids” Rev. Mod. Phys., 90(1), 015001

[2] Z. Li, Y. Zeng, J. Zhang, M. Zhou and W. Wu (2018) “Observation of negative longitudinal magnetoresistance in the type-II Dirac semimetal PtSe2” Phys. Rev. B, 98(2), 165441

#110	THU	COND 4	17:00 – 17:15	HS 9

$EuCd_2X_2$: Semimetal illusion versus Semiconductor reality

S. Nasrallah[1,2*], D. Santos-Cottin[1], F. Le Mardele[3], J. Wyzula[1], I. Mohelsky[1], J. Barrett[1,6], W. Galloway[1,6], I. Zivkovic[5], L. Aksamovic[2], P. Sacer[4], M. Novak[4], N. Barisic[2,4], C. C. Homes[7], M. Orlita[3,8], and A. Akrap[1*]

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The search for intrinsic magnetic topological materials has captured the interest of numerous scientists in recent years due to their potential spintronic application. $EuCd_2X_2$ (X = Sb, As, P) family was predicted by Density Functional Theory (DFT) to be a topological, Weyl semimetal [1-2]. This claim was further supported by transport measurements and Angle-Resolved Photoemission Spectroscopy (ARPES), which exhibited metallic-like resistivity and the conical shape of the valence band, respectively [3-4].

However, our recent infrared- and magneto-optics measurements revealed that $EuCd_2X_2$ is a magnetic semiconductor rather than a topological Weyl semimetal. We obtained energy gaps of 0.5 eV, 0.77 eV, and 1.2 eV for X = Sb, As, and P, respectively [5] [6]. These band gaps are notably influenced by the application of a magnetic field, undergoing redshifts of 45 meV, 125 meV, and 150 meV, respectively. Despite these shifts, magneto-optics shows that the band gaps do not close even under the application of a high field of 35T, indicating that the compounds remain semiconductors and thus excluding a magnetic Weyl semimetal scenario.

Additionally, ARPES and pump-probe ARPES on $EuCd_2As_2$ confirmed the band gap of 0.7 eV. The resistivity measurements revealed activation behavior for $EuCd_2As_2$ and $EuCd_2P_2$, while $EuCd_2Sb_2$ exhibited metallic-like resistivity, implying that the system is doped.

In conclusion, our study provides valuable insights into the effects of element substitution on the electronic band structure of $EuCd_2X_2$ semiconductors.

[1] G. Hua et al., Physical Review B 98, 201116 (2018).
[2] H. Su et al., APL Materials 8, 011109 (2020).
[3] Y. Shi et al., Physical Review B 109, 125202 (2024)
[4] J. Ma et al., Advanced Materials 32, 1907565 (2020)
[5] D. Santos-Cottin et al., Physical Review Letters 132, 186704 (2023)
[6] S. Nasrallah et al., unpublished

#111	THU	PIN 2	17:00 – 17:30	HS 10

Fire Safety Research – Stumblin' In

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I studied physics at JKU Linz, completing both my diploma and PhD at the Institute of Semiconductor and Solid State Physics. In those years a was concerned with "Growth and characterization of organic semiconductors". However, this will not be the focus of my contribution. Instead, I will provide an overview of my journey into fire safety research.

A few days after defending my phd on March 5, 2013, I found a job advertisement on my desk. I decided to apply, and half a year later, I started at IBS. My initial focus was on performing computational fluid dynamics (CFD) simulations of fire. The goal of these simulations is to gather information about heat and smoke distributions in the event of a fire. This information is crucial for tailoring the safety features of a building.

To perform my job effectively, I had to learn a lot about fire safety. Consequently, I expanded my work from CFD simulations to various areas within the company, including building inspections and post-fire investigations.

As a physicist, I am always interested in exploring new things. This led me to draft and manage research projects, which ranged from the "development of CFD/FEM simulations for fire resistance tests" to more down to earth topics like "How does the fire behavior of foil roofs change when PV systems are present?" The latter might not be "high-level science", but it's fun to burn stuff. Additionally, the results formed the basis for updated building regulations. Such regulations may sound boring, but they allowed the utilization of industrial roofs for PV installations without facing legal liabilities and conflicts with building regulators and insurance companies. This is a big deal for large scale PV-application on industrial buildings.

All those experiences finally led me to represent our company as a press officer and to work in the executive team.

What I want to coney is that careers offer many unexpected opportunities, and I would advise to (sometimes) try things out and see where the path leads you.

#112	MON	COND 4	17:15 – 17:30	HS 9

Influence of thermally activated orbitals on conductivity in correlated materials

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We present model calculations to study the effect of thermally activated electrons on the resistivity of strongly correlated materials with temperature. The results are obtained through dynamical mean-field theory calculations of a degenerated two-orbital Hubbard-Kanamori model and a similar three-orbital model, where we allow electrons to be thermally excited into the additional orbital. We find that for intermediate to high interaction strengths, the resistivity drastically increases when the additional orbital is being populated. We argue that the main reason for this are stronger correlations, that arise because the system slowly approaches half-filling. These correlations increase electron-electron scattering that dominates resistivity in correlated materials. Because of the high scattering rates and the comparatively low electron density in the additional orbital, the high resistivity is mainly due to the increased correlations in the base orbitals when the additional orbital is present. We furthermore argue that our findings can be linked to a gradual spin-crossover (SCO), a claim backed by the non-monotonicity of the local magnetic susceptibility. With this in mind, we discuss the applicability of our model to real materials, where MOFs exhibiting SCO seem most promising. Overall, we provide insight into how electronic correlations affect the link between spin-crossover and resistivity.

#113	THU	PIN 2	17:30 – 18:00	HS 10

Physik & Wirtschaft – ein Widerspruch ?

P. Schwab[1]

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Der Physiker Peter Schwab, ein Absolvent der JKU, war mehr als 30 Jahre in der voestalpine, einem internationalen Stahl- und Technologiekonzern tätig. Er erzählt wie er vom einfachen Forschungsingenieur über mehrere Stationen zum Forschungschef und schlussendlich zum Vorstand des Konzerns aufstieg. Dort verantwortete er die Metal Forming Division mit einem Umsatz von knapp 4 Mrd. Euro, rund 12.000 Mitarbeitern und zahlreichen produzierenden Unternehmen in Europa, Nord- und Südamerika, Südafrika und China. Anhand der einzelnen Karriereschritte erläutert er welche Eigenschaften und Fähigkeiten es für eine derartige Karriere braucht und warum die Ausbildung zum Physiker sehr hilfreich dabei war.

Abstracts

SFB BeyondC talks

#114	THU	SFB BeyondC	14:00 – 14:30	BA 9911

How to fault-tolerantly realize any quantum circuit with local operations

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We show how to realize a general quantum circuit involving gates between arbitrary pairs of qubits by means of geometrically local quantum operations and efficient classical computation. We prove that circuit-level local stochastic noise modeling an imperfect implementation of our derived schemes is equivalent to local stochastic noise in the original circuit. Our constructions incur a constant-factor increase in the quantum circuit depth and a polynomial overhead in the number of qubits: To execute an arbitrary quantum circuit on n qubits, we give a 3D quantum fault-tolerance architecture involving O(n^{3/2}\log^3 n) qubits, and a quasi-2D architecture using O(n^2 \log^3 n) qubits. Applied to recent fault-tolerance constructions, this gives a fault-tolerance threshold theorem for universal quantum computations with local operations, a polynomial qubit overhead and a quasi-polylogarithmic depth overhead. More generally, our transformation dispenses with the need for considering the locality of operations when designing schemes for fault-tolerant quantum information processing.

This is joint work with Shin Ho Choe, arXiv:2402.13863

#115	THU	SFB BeyondC	14:30 – 15:00	BA 9911

PaQS: The Paderborn Quantum Sampler

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Gaussian Boson Sampling (GBS) has advanced rapidly since its inception and subsequent full-scale demonstrations. Not only has GBS provided the most compelling evidence of quantum computational advantage, but many possible applications are now being explored, such as calculating vibronic spectra and drug discovery algorithms.

A GBS system consists of squeezed state generation, a linear optical network, and high efficiency photon number resolved detection. Although the core components remain constant, any experimental realisation will implement these components in varying ways due to trade-offs inherent in their design principles. For example, full programmability typically comes at the cost of increased losses, while time-multiplexed interferometers are typically sensitive to fibre dispersion and thus require narrowband squeezed light sources, necessitating the use of optical cavities.

Here, we present the Paderborn Quantum Sampler (PaQS), the functioning GBS architecture constructed at Paderborn University, which has been designed with a view towards full integration. The required squeezed states are produced in a single periodically poled potassium titanyl phosphate waveguide chip through a time-multiplexing scheme. This design allows for single-pass generation of up to 16 squeezed states with high efficiencies, enabling the production of squeezed states with extremely high average photon number (above 1000). The fully integrated interferometer provides complete programmability of any 12-mode unitary. The 12 output channels of the interferometer are detected on separate SNSPDs with demonstrated intrinsic photon number resolution.

PaQS provides an ideal platform for exploring the benefits and challenges of time-multiplexed, waveguided source generation and system integration in GBS experiments. Furthermore, the source design allows for investigations in the high photon number regime while the fully programmable interferometer provides the means to explore other protocols beyond the standard GBS scheme.

#116	THU	SFB BeyondC	15:00 – 15:30	BA 9911

Generating quantum circuits with diffusion models

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We show how to realize a general quantum circuit involving gates between arbitrary pairs of qubits by means of geometrically local quantum operations and efficient classical computation. We prove that circuit-level local stochastic noise modeling an imperfect implementation of our derived schemes is equivalent to local stochastic noise in the original circuit. Our constructions incur a constant-factor increase in the quantum circuit depth and a polynomial overhead in the number of qubits: To execute an arbitrary quantum circuit on n qubits, we give a 3D quantum fault-tolerance architecture involving O(n^{3/2}\log^3 n) qubits, and a quasi-2D architecture using O(n^2 \log^3 n) qubits. Applied to recent fault-tolerance constructions, this gives a fault-tolerance threshold theorem for universal quantum computations with local operations, a polynomial qubit overhead and a quasi-polylogarithmic depth overhead. More generally, our transformation dispenses with the need for considering the locality of operations when designing schemes for fault-tolerant quantum information processing.

This is joint work with Shin Ho Choe, arXiv:2402.13863

#117	THU	SFB BeyondC	16:00 – 16:30	BA 9911

BruQner – The Sound of Entanglement

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Anton Bruckner's work has made music history and is known far beyond the country's borders. Austria is also internationally known for its contributions to quantum physics. In “BruQner” these two worlds meet – on September 4th, 2024, in the New Cathedral in Linz. Using a musical interpretation of a Bell test, striking passages from Bruckner's work are made audible in a new way. A sensual symbiosis of music, visuals and modern research is created. “BruQner” is one of the first attempts in the world to work musically with entanglement. Entangled photon pairs from lasers take on the role of a “quantum conductor” and allow the two cathedral organists to play music which no human conductor or classical computer could instruct. This talk will give an overview of the development of this project and the event itself.".

#118	THU	SFB BeyondC	16:30 – 17:00	BA 9911

AI, Machine Learning, and the Human Element in Music

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Music is a wonderful thing, and a complex manifestation of human intellect and creativity. It is also a wonderful object of study for a discipline that calls itself Artificial Intelligence. We will look at some recent AI research that focuses on a central and "deep" aspect of music: its expressivity, and how performers can make it expressive through their playing. You will also be subjected to a little experiment which may, or may not, yield a surprising result. No "quantum" of any kind involved.

Abstracts

Poster session

P01	TUE	AKCP	14:00 – 15:30	HS 17

Working Group for Equal Opportunities (Arbeitskreis für Chancengleichheit in der Physik – AKCP): Where do we stand? Where do we want to go?

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Founded by Professor Günther Bauer back in 1992, the Working Group for Equal Opportunities in Physics (Arbeitskreis für Chancengleichheit in der Physik – AKCP) of the Austrian Physical Society aims at making female physicists more visible and thus increasing the equal opportunities for them at universities and in the private sector.

Despite the relatively high number of female students in physics (30.3% in Bachelors´ degree in 2023), the number of women decreases the further they progress in their academic careers. This shows a particularly high need for improvement for women in physics with regard to careers and promotion opportunities: the average number of female professors and associate professors at Austrian universities is around 12% (as of 2023).

After a seven-year break, the AKCP was reactivated in September 2023 with the task to make awareness of the inequal opportunities that exist in physics. Here we show the state of the art of gender inequality in Austrian universities and propose measures to improve the current situation. Although equal opportunities and gender equality in physics have improved in recent decades, there is still a long way to go before achieving real equal opportunities.

P02	TUE	AMP	14:00 – 15:30	HS 17

Discrimination of technical polymers by Laser-Plasma-Spectroscopy

L. Lang[1], N. Giannakaris[1], S. Grünberger[1,2], and J. D. Pedarnig[1]

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Technical polymers are produced in large quantity (nine billion tons in total until 2017) - and only an estimated 10% of the plastic waste generated so far has been recycled [1]. New technologies for the discrimination of polymers may contribute to more efficient and effective recycling. We combine Spark optical emission spectroscopy (OES) and Laser-induced breakdown spectroscopy (LIBS) to discriminate different polymers. Both techniques are used for element analysis in various industry branches [2]. A laser pulse is applied to a polymer sample inducing faint plasma, followed by an electric spark discharge between two electrodes. The optical emission of plasma is analyzed (Laser Ablation-Spark Discharge-OES, LA-SD-OES). Different technical polymers (PA6, PC, PE-HD, PET, PMMA, POM, PP, PS, PTFE, PVC, UHMWPE, etc.) are measured by LIBS and LA-SD-OES. Molecular emission band of C2 and atomic emission lines of O, N, and H are measured and the correlation of intensities is used for materials discrimination. LA-SD-OES outperforms LIBS, especially for polymers containing halogens. Various gas flows are introduced to minimize the influence of the surrounding atmosphere and to improve the distinguishability of the technical polymers.

Acknowledgments: Financial support by the Austrian Research Promotion Agency FFG is gratefully acknowledged (K-project PSSP 871974, COMET Competence Center CHASE GmbH K1-Center 868615).

[1] R. Geyer, "Production, use, and fate of synthetic polymers", in Plastic Waste and Recycling, pages 13-32, (Ed.: T.M. Letcher), Academic Press (2020).

[2] J.D. Pedarnig, S. Trautner, S. Grünberger, N. Giannakaris, S. Eschlböck-Fuchs, J. Hofstadler, "Review of Element Analysis of Industrial Materials by In-Line Laser-Induced Breakdown Spectroscopy (LIBS)", Applied Sciences 11 (2021) 9274.

P03	TUE	AMP	14:00 – 15:30	HS 17

Surface Cleaning with Atmospheric Pressure Plasma Jets investigated by in-situ Optical Emission Spectroscopy and by LIBS chemical imaging

J. D. Pedarnig[1], M. Niebauer[1], N. Giannakaris[1], G. Gürtler[1,2], and T. Stehrer[3]

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Atmospheric pressure plasma jets (APPJs) are employed for surface cleaning, modification of surfaces, deposition of coatings. etc. We investigate the plasma of an industrial APPJ (Acerios, Fronius International GmbH) and apply it to the cleaning of contaminated metals. The device operates a spark discharge in Argon gas flow resulting in a continuous plasma jet of kW power expanding into ambient air (Fig. 1, left). The plasma parameters are measured by Optical emission spectroscopy (OES) [1]. For surface cleaning the samples are coated with oil layers of 0.5 µm to 10 µm thickness. The plasma cleaning is monitored in-situ by OES and ex situ by chemical imaging using Laser-induced breakdown spectroscopy (LIBS). The APPJ plasma cleaning efficiency is calculated from measured spectra and the intensities of atomic lines and molecular bands of species originating from the contamination layer. Spatial profiles of the cleaning efficiency are measured by LIBS (Fig. 1, right). We find a strong influence of the plasma parameters and of the type and thickness of contamination layer on the APPJ cleaning efficiency [2]. For instance, cleaning becomes more efficient at higher power of the plasma generator (CN violet band emission measured in situ by OES).

Acknowledgments: Financial support by the Austrian Research Promotion Agency FFG is gratefully acknowledged (project CAPCOAT Plus 872846).

[1] N. Giannakaris, G. Gürtler, T. Stehrer, M. Mair, J.D. Pedarnig, "Optical Emission Spectroscopy of an industrial thermal Atmospheric Pressure Plasma Jet: Parametric Study of Electron Temperature", Spectrochim. Acta Part B 207 (2023) 106736.
[2] N. Giannakaris, M. Niebauer, et al., "Surface Cleaning with APPJ monitored in-situ by Optical Emission Spectroscopy" (to be submitted 2024).

P04	TUE	AMP	14:00 – 15:30	HS 17

Solution of the Hypernetted-Chain-Euler-Lagrange Equation for a Bose Gas using a new Phase Shift Method

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In experiments, the scattering length of Bose gases can be adjusted via magnetic Feshbach resonances. In calculations, this is usually described by model potentials rather than scattering phase shifts. In this work we treat the many body problem numerically with a variational method, the hypernetted-chain Euler-Lagrange method, directly using the phase shift instead of a model potential. We restrict ourselves to homogeneous Bose gases which can be realised experimentally in box traps [1]. Using imaginary time propagation we obtain the ground state energy and the pair distribution function and compare with results obtained using a model potential. Both methods give the same results, but the new phase shift method is much more efficient, allowing significantly larger imaginary time steps. Our new method also works for interactions supporting two-body bound states which are effectively projected out during time evolution. In future investigations we want to study the many body dynamics caused by time dependent interactions such as interaction quenches [2]. This is done by implementing the phase shift method for the *time dependendent* hypernetted-chain Euler-Lagrange method [3].

[1] N. Navon , R. P. Smith, Z. Hadzibabic, Nat. Phys. 17, 1334-1341 (2021).

[2] R. J. Fletcher, R. Lopes, J. Man, N. Navon, R. P. Smith, M. W. Zwierlein, and Z. Hadzibabic, Science 355, 377 (2017).

[3] M. Gartner, D. Miesbauer, M. Kobler, J. Freund, G. Carleo, R. E. Zillich, arXiv:2212.07113v1 (2022).

P05	TUE	AMP	14:00 – 15:30	HS 17

Preferential Adsorption and Kondo Signature of spin-$^1/_2$ radical molecule BDPA on Cu(100)

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The adsorption of the radical α,γ-bisdiphenylene-β-phenylallyl (BDPA) molecule to a Cu(100) surface was studied using scanning tunnelling microscopy (STM), scanning tunnelling spectroscopy (STS), and density functional theory which accounts for dispersion forces (DFT-vdW). The adsorption of BDPA on Cu(100) was observed to have an epitaxial fit preference for $\langle 01\bar{1} \rangle$ directions due to weak Cu-C chemisorption between fluorenyl carbons and the underlying copper atoms. The bean shape of the BDPA molecule on Cu(100) can be ascribed to the lack of molecular orbital character on the phenyl substituent, and Kondo-like features observed in differential conductance (dI/dV) measurements suggest the retention of a S=½ spin state. This is supported by DFT-vdW, which predicts a singular unpaired electron in the distorted adsorption structure of the BDPA.

P06	TUE	AMP	14:00 – 15:30	HS 17

Laser-induced surface structures as substrates for cell alignment or repellence

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This paper describes methods for achieving directed growth of Schwann cells, a type of glial cells that can support the regeneration of the nerve pathway by guiding the neuronal axons in the direction of their alignment [1], or the repellence of osteoblasts, which build up bones, from the surface of materials of bone implants [2]. These methods imply the exposure of a substrate, typically a titanium alloy or a hard polymer material, to a linearly polarized pulsed femtosecond laser beam at a wavelength of 1040 nm, that generates laser-induced periodic surface structures (LIPSS) with a periodicity of a few hundred nanometers. For both cell types, we show that the cells grow in a certain direction, predetermined by nanoripples orientation. In contrast, cells cultivated onto unstructured surfaces, show an omnidirectional growth behavior. At higher laser fluences and pulse numbers, the irradiation of titanium alloy surfaces induces the formation of steep micrometer-scale spikes which are still covered with LIPSS. This hierarchical combination of laser-induced micro- and nanostructures can lead to the repellence of osteoblasts seeded thereon, which is promising for applications where medical implants must be removed a certain time after implantation.

References:

[1] S. Lifka, C. Plamadeala, A. Weth, J. Heitz, and W. Baumgartner, Open Research Europe 4, 80 (2024);

[2] M. Muck, B. Wolfsjäger, K. Seibert, C. Maier, S.A. Lone, A.W. Hassel, W. Baumgartner, and J. Heitz, Nanomaterials 11, 1342 (2021)

P07	TUE	COND	14:00 – 15:30	HS 17

Temperature-dependent Raman spectroscopic characterization of poly (furfuryl alcohol)

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Recently we employed FTIR spectroscopy and Raman spectroscopy to investigate the chemical constitution of the polymer polyfurfuryl alcohol (PFA) synthetizes in different ways, and appearing macroscopically different: the first one being a liquid and viscous commercial sample, the second one being a self-prepared solid and rigid sample, produced following a thermosetting procedure. As a continuation of the research activities dealing with thermosetted PFA, we have additionally performed a set of temperature dependent Raman spectroscopic measurements in order to study the evolution of these Raman spectra during the glass transition of thermosetted PFA, adopting a similar spectral analysis previously performed to infer about the glass transition of the polymer poly(methyl methacrylate) (PMMA), including analysis of the Raman spectra by two-dimensional correlation spectroscopy (2DCOS).

At the University of Salzburg the Raman measurements were performed in the temperature range between -160°C and +300°C with laser excitation in the blue spectral range at 455 nm, while at the IUVSOFF beamline of the Elettra synchrotron in Trieste a series of Resonant Raman measurements were performed in the UV spectral range with laser excitation at 266 nm.

Compatible with the Differential Scanning Calorimetry (DSC) data recorded from 10° C to 180°C for the thermosetted PFA, resulting in a glass transition temperature at around 82°C, the Raman spectroscopic spectral features of the thermosetted PFA also change with temperature in the temperature range at around 82°C, this spectral evolution being also a clear indication of structural changes taking place during the glass transition of thermosetted PFA.

P08	TUE	COND	14:00 – 15:30	HS 17

Spin pumping into a partially compensated antiferromagnetic/paramagnetic insulator

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The field of spintronics requires the controlled generation and detection of magnetization dynamics. In ferromagnetic / non-ferromagnetic (FM/NM) heterostructures such magnetization dynamics can be generated via spin pumping which is a flow of angular momentum into the NF generated by the precessing magnetization of the FM resulting in an increased Gilbert damping parameter □. Insulating materials have the advantage that an eventually increased magnetic damping is less influenced by other mechanisms like eddy-current damping. Therefore, heterostructures of insulating Co-substituted ZnO (Co:ZnO) as NF and metallic Permalloy (Py) as FM have been investigated for their static and dynamic magnetic interactions. Initially, multi-frequency ferromagnetic resonance (FMR) has indicated the presence of spin pumping from Py into the paramagnetic phase of Co:ZnO at 300 K [1]. This was corroborated by element selective measurements using time-resolved scanning transmission x-ray microscopy evidencing a dynamic magnetic contrast at the Co-edge which was antiphase to the one of the Py [2]. Temperature-dependent conventional X-band FMR has further demonstrated a maximum of the FMR linewidth around the para- to antiferromagnetic transition temperature of Co:ZnO [1]. Here we show temperature-dependent, broad-band FMR experiments on Py/Co:ZnO heterostructures across the magnetic phase transition which allow to separate the various contributions to the FMR line-width and thus to extract the temperature-dependence of α. We find a significant increase of α(T) around the magnetic phase transition of Co:ZnO which confirms spin pumping into the fluctuating spin sink of an antiferromagnetic/paramagnetic insulator [3].

[1] M. Buchner et al., J. Appl. Phys. 127 (2020) 043901
[2] S. Pile et al., Phys. Rev. Applied 14 (2020) 034005
[3] M. Buchner et al., New J. Phys. 25 (2023) 073002

P09	TUE	COND	14:00 – 15:30	HS 17

Concepts for Predicting Phase Transition

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Phase transitions, described by the (Helmholtz) free energy F are mainly governed by thermodynamic extensive quantities like (binding) energy and entropy, and by further terms like the sored magneto-static or electro-static energies, or volume, strain energy or surface contributions, or intensive quantities as e.g., pressure or temperature. Electromagnetic fields respectively photons do not enter this balance. Knowing the different phases with the respective Helmholtz energy one can predict the order and the condition for the phase transition. With this model one has the tools to investigate and adjust the transition for practical application. A more fundamental approach is to use quantum mechanic for finding the properties and condition for the phase transitions. In this approach the driving force for the phase transitions is the electron-phonon coupling.

To model this phase transition in mathematical detail, we use the Hamiltonian suggested by Kristoffel et al. [1]:

$$\hat{\mathrm{H}} = \underbrace{\sum_{\vec{q}j}\left(\frac{1}{2M_j}P_{\vec{q}j}P_{-\vec{q}j} + \frac{M_j}{2}\omega_{\vec{q}j}x_{\vec{q}j}x_{-\vec{q}j}\right) + \sum_{\vec{q}_1 j_1}\sum_{\vec{q}_2 j_2}\sum_{\vec{q}_3 j_3}\sum_{\vec{q}_4 j_4} B(\vec{q}_1 j_1, \vec{q}_2 j_2, \vec{q}_3 j_3, \vec{q}_4 j_4) x_{\vec{q}_1 j_1} x_{\vec{q}_2 j_2} x_{\vec{q}_3 j_3} x_{\vec{q}_4 j_4}}_{\hat{\mathrm{H}}_{\mathrm{p}}} + \hat{\mathrm{H}}_{\mathrm{hI}}$$

$$+ \underbrace{\sum_{\sigma,\vec{k}} \varepsilon_\sigma(\vec{k}) \hat{a}^\dagger_{\sigma\vec{k}} \hat{a}_{\sigma\vec{k}}}_{\hat{\mathrm{H}}_{\mathrm{e}}} + \hat{\mathrm{H}}_{\mathrm{e\text{-}e}} + \underbrace{\frac{1}{\sqrt{N}} \sum_{\sigma\sigma'} \sum_{\vec{k},\vec{k}'} \sum_{\vec{q}j} V^j_{\sigma\sigma'}\left(\vec{q},\vec{k},\vec{k}'\right) \hat{a}^\dagger_{\sigma\vec{k}} \hat{a}_{\sigma'\vec{k}'} \delta\left(\vec{k}' - \vec{k} + \vec{q}\right) x_{\vec{q}j}}_{\hat{\mathrm{H}}_{\mathrm{p\text{-}e}}} + \hat{\mathrm{H}}_{\mathrm{h\text{-}p\text{-}e}}$$

The Hamiltonian contains two sub-systems, namely the phononic one (first two terms in the 1st line represent the harmonic contribution, the third one the first two anharmonic and the last term includes higher phononic terms) and the electronic one (first two terms in the 2nd line). These interact with each other via $\hat{H}_{p-e}$, describing the electron-phonon coupling (2nd line, last two terms with linear and higher coupling). With such a Hamiltonian and concepts derived by Landau-Lifshitz one can determine the order of the phase transition and the physical key parameters and learn, how to modify the transition.

1. Kristoffel, N., & Konsin, P. (1988). Vibronic Theory of Structural Phase Transitions and Displacive Ferroelectrics. Physica Status Solidi (B), 149(1), 11–40.

P10	TUE	COND	14:00 – 15:30	HS 17

Temperature dependence of relativistic valence band splitting induced by an altermagnetic phase transition

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Altermagnetic (AM) materials can exhibit non-relativistic, momentum-dependent spin-split states, ushering in new opportunities for spin electronic devices [1-3]. While the characteristics of spin-splitting have been documented within the framework of the non-relativistic spin group symmetry, there has been limited exploration of the inclusion of relativistic symmetry and its impact on the emergence of a novel spin-splitting in the band structure. This study delves into the intricate relativistic electronic structure of an AM material, α-MnTe. Employing temperature-dependent angle-resolved photoelectron spectroscopy across the AM phase transition, we elucidate the emergence of a relativistic valence band splitting concurrent with the establishment of magnetic order [4]. This discovery is validated through disordered local moment calculations, modeling the influence of magnetic order on the electronic structure and confirming the magnetic origin of the observed splitting. The temperature-dependent splitting is ascribed to the advent of relativistic spin-splitting resulting from the strengthening of AM order in α-MnTe as the temperature decreases. This sheds light on a previously unexplored facet of this intriguing material.

[1] L. Šmejkal, J. Sinova, T. Jungwirth, Phys. Rev. X. 2022, 12, 011028.
[2] L. Šmejkal, J. Sinova, T. Jungwirth, Phys. Rev. X. 2022, 12, 040501.
[3] J. Krempaský, L. Šmejkal, S. W. D'Souza, M. Hajlaoui, et al. Nature 2024, 626, 517.
[4] M. Hajlaoui, S. Wilfred D'Souza, L. Šmejkal, et al. Adv. Mater. 2024, 2314076.

P11	TUE	COND	14:00 – 15:30	HS 17

Electrically conductive, sub-micron sized organic wires made from Polypyrrole

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Organic electronics represents a rapidly expanding field characterized by its unique properties, including flexibility, low cost, biocompatibility and tunability. These offer significant advantages over its well-established inorganic counterparts. This versatility enables their excellence in applications such as wearable electronics, sensors, particularly biosensors, and various other, especially low-power devices [1].

However, the micromanufacturing of organic electronics presents a challenge due to limited compatibility with established patterning techniques designed for inorganic materials, such as UV or e-beam lithography. Innovative approaches employing red photons of low quantum energies are thus imperative to tailor manufacturing processes to accommodate and utilize these distinctive properties for more efficient patterning.

This study presents a novel method for producing sub-micron-sized organic wires. By scanning a femtosecond laser over liquid pyrrole, we induce multiphoton absorption, leading to polymerization and the formation of solid wires. This process enables rapid production of miniature electronic structures in customizable patterns, facilitating the development of fast and flexible electronics [2]. Additionally, the process can be enhanced by incorporating photo starters like 7-diethylamino-3-thenoylcoumarin (DETC) or dopants to optimize the results for specific applications, potentially allowing the production of semiconductor structures such as diodes or transistors.

The produced wires exhibit widths of less than a micron and heights of less than 50 nanometers, maintaining consistency across lengths of at least 200 microns when characterized with an AFM. They demonstrate a specific conductivity of 100 S/cm and exhibit characteristics of an ohmic resistor in 4-probe measurements.

References

[1] Yang, Xi, and Liming Ding. "Organic semiconductors: commercialization and market." *J. Semicond* 42.9 (2021): 090201.

[2] Shuyu Liang, Ying Yang, Chao Lv, Yuefeng Liu, and Hong Xia, "Integratable photodetectors based on photopolymerized conductive polymer via femtosecond laser direct writing," Opt. Lett. 47, 2630-2633 (2022)

P12	TUE	COND	14:00 – 15:30	HS 17

Mode analysis of partially spin- and valley-polarized electron layers

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Electrons in multi-component (quasi-)two-dimensional layers, such as realized in semiconductor heterostructures or graphene, show a multitude of collective excitations with promising applications in advanced electronic and optoelectronic devices. Many materials exhibit well separated local minima in their band structure, called “valleys”. Their occupation, controllable by external strain, can often be modeled by a quasi-spin. If both, the number of spin-up and spin-down electrons as well as that of electrons in the two relevant valleys differ, this four-component many-body system exhibits four different types of plasmons. The common charge plasmon is an in-phase movement of all electrons, the spin-plasmon (valley-plasmon) is characterized by an opposite oscillation of the spin (valley) carriers. For the remaining mode the product of spin and quasi-spin is relevant. Between these modes three anti-resonances are found, where all single-particle and collective excitations are suppressed. An accurate prediction of all these dispersions to harness their specifics for spintronic and valleytronic applications requires a comprehensive mode analysis.

We here investigate the plasmons in GaAs/AlGaAs quantum wells. For the purely spin-polarized case, experimentally studied in Ref.[1], we use effective interactions [2] based on high-quality static structure Monte Carlo data. At very high dilutions an incipient soft mode near the phase transition to a Wigner crystal goes in hand with a flip in mode-flavor from charge-like to spin-like character. In the four-component spin- and valley-polarized system we account for the electrons' correlations by modified Hubbard local field corrected potentials Fig.6.9.c above). knowing the [3]. Where the three linear modes come close, mode-repulsion results in drastic change of the mode flavor near this wave vector, strongly influencing the excitation behavior of the system.

[1] C.F. Hirjibehedin, A. Pinczuk, B.S. Dennis, et al. Phys. Rev. B **65**, 161309 (2002).
[2] D. Kreil, R Hobbiger, J.T. Drachta, et al. Phys. Rev. B **92**, 205426 (2015)
[3] M. Schober, Master’s thesis, Johannes Kepler University, Linz, Austria (2021)

P13	TUE	COND	14:00 – 15:30	HS 17

Emerging Multiferroic Properties in Defective Perovskite Oxides

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Ferroelectricity, a functional material property, emerges through various mechanisms, each offering unique pathways toward polarization. Conventional second-order Jahn-Teller polarization in ferroelectric perovskite oxides, and strain engineering in thin films are among the diverse methods employed to achieve this phenomenon. Moreover, single-phase materials that exhibit both ferroelectric and magnetic properties above room temperature are highly desirable, sparking ongoing research into unconventional ferroelectric mechanisms in magnetic oxides.

Here, we investigate an underexplored route towards ferroelectricity by introducing antisite defects in the perovskite oxide $LaFeO_3$. Our density functional theory (DFT) calculations uncover a highly non-centrosymmetric environment of a Fe_{La} antisite defect that leads to switchable ferroelectricity.

Our findings not only highlight the potential of rendering the antiferromagnet $LaFeO_3$ ferroelectric and thus multiferroic but also offer valuable insights for the broader field of defect-engineered functional materials. By establishing a novel method to achieve ferroelectricity, this research opens avenues for tailored functional material properties for advanced electronic applications. Ultimately, this study emphasizes the significance of defect engineering as a powerful tool for rational material design and optimization.

P14	TUE	COND	14:00 – 15:30	HS 17

Progress in STED-inspired sub-diffractional lithography of epoxides

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The past two decades have seen substantial advancements in direct laser writing by two-photon lithography, enhanced by techniques adapted from stimulated emission depletion (STED) microscopy.[1] Initially, STED-inspired lithography was predominantly applied to radical polymerizations, especially with acrylates and methacrylates,[2] while cationic polymers, particularly epoxides, crucial in semiconductor clean-room technology, did not benefit from this method.

Recently, we investigated a resist comprising 3,4-epoxycyclohexylmethyl 3,4 epoxycyclohexanecarboxylate (EPOX) as monomer, triarylsulfonium hexafluoroantimonate salt as starter and 2-isopropylthioxanthone (ITX) as a photo-sensitizer. Using a 780 nm femtosecond laser for two-photon excitation and a 660 nm continuous wave laser for depletion, we achieved 125 nm structure sizes.[3] Utilizing 2-chlorothioxanthone (CTX) instead of ITX, allowed for writing feature sizes down to 83 nm.[4], which is roughly l/10 of the excitation wavelength. This holds promise of delivering feature sizes on par with those obtained in acrylate polymerization[5].

In this contribution, we will present our latest progress on STED-inspired lithography of epoxides.

1. Klar, T. A.; Hell, S. W., Subdiffraction resolution in far-field fluorescence microscopy. Opt. Lett. 1999, 24 (14), 954-956.

2. Fischer, J., & Wegener, M. Three-dimensional optical laser lithography beyond the diffraction limit. Laser & Photonics Reviews, 7(1), 22–44 (2012).

3. S. Islam, M. Sangermano, and T. A. Klar, "STED-Inspired Cationic Photoinhibition Lithography," Journal of Physical Chemistry C 127, 18736−18744 (2023).

4. S. Islam, and T. A. Klar, “STED-inspired sub-100 nm structuring of epoxides using CTX as photosensitizer”, ACS Omega 2024 9 (17), 19203-19208.

5. Gvindzhiliia et al. ACS Appl. Optical Mater.1, 945, 2023.

P15	TUE	COND	14:00 – 15:30	HS 17

Influence of oxidic and metallic interfaces on the magnetic damping of Permalloy thin films

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The understanding of magnetic damping in ferromagnetic (FM) materials is of high importance from a fundamental point of view. To quantify the magnetic damping in ferromagnetic resonance (FMR), the Gilbert damping parameter α [1] is the central quantity. However, a fundamental understanding of all relevant mechanisms contributing to the magnetic relaxation is still lacking. Permalloy ($Ni_{80}Fe_{20}$, Py) is a very suitable FM metal to study magnetic damping mechanisms because its fundamental magnetic properties are well understood. Nevertheless, the available data for α spreads over the range of $4 - 9 \times 10^{-3}$ [2]. Since Py is a model system of a metallic FM with low magnetic damping, a systematic study of the environment of Py is required for a better understanding and control of the intrinsic magnetic damping. Here, we report on 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 different materials suitable for preventing oxidation (Ta, Al, and SiOx). The resulting frequency and temperature dependence of the FMR linewidth significantly deviates from the expected Gilbert-like behavior and especially for oxidic interfaces unwanted non-Gilbert-like contributions to the magnetic damping appear, in particular, at low temperatures [3]. In contrast, metallic capping layers avoid non-Gilbert-like contributions. In particular, Py sandwiched in between Al metallic capping and buffer layers exhibits negligible inhomogeneous FMR linewidth broadening and a very small, purely Gilbert-like contribution of α = 0.0066(2) down to the lowest temperature [3].

[1] T. L. Gilbert, IEEE Trans. Magn. **40** (2004) 3443
[2] A. A. Starikov et al., Phys. Rev. Lett. **105** (2010) 236601; M. A. W. Schoen et al., Phys. Rev. B **95** (2017) 134411
[3] V. Ney et al., Phys. Rev. Materials **7** (2023) 124403

P16	TUE	COND	14:00 – 15:30	HS 17

Optimizing Laser-Induced Phase Transformations in Sb_2S_3 Thin Films: Simulation Framework and Experiments

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We present a comprehensive simulation framework for modeling laser-induced amorphization in phase-change material (PCM) thin films, with a focus on Sb_2S_3. Our model incorporates critical factors such as thin film interference, heat transfer, and melting-induced changes in optical properties. We validate the simulations through picosecond laser amorphization experiments and Raman spectroscopy analysis. The framework enables rapid optimization of film thickness and laser parameters to maximize energy efficiency, melting effectiveness, and quenching rates. This study provides fundamental insights into Sb_2S_3 laser amorphization dynamics and offers a powerful tool for simulation-guided optimization of PCMs for photonic applications.

P17	TUE	COND	14:00 – 15:30	HS 17

A multi-technique thorough synthesis and characterization of tannin-furanic foams, a sustainable biobased alternative to foams derived from fossil fuel-based chemicals

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Aiming on sustainability options, materials that are discarded from the industry, and given a second life, are highly desirable. In particular, discovering a comparable green alternative to polyethylene terephthalate or polystyrene could represent a great breakthrough in diminishing global plastic waste. Condensed tannins, extracted from the saw-mill residue bark, constitute the starting point to create tannin-furanic foams, a rigid biobased material that could be a sustainable alternative to those derived from fossil fuel-based chemicals.

With the aim of developing novel foam production strategies, three tannin-furanic foams, namely *mechanical*, *sulfuric* and *nitric* (their synthesis differing by changing chemical formulation and foaming process), were thoroughly chemically characterized, and their morphological and macroscopic properties were compared with those of commercial plastic foams made of polystyrene and of polyethylene terephthalate. Understanding the influence of the foaming method on the foam properties is of utmost importance when aiming to substitute existing, well-established products.

The chemical characterization was performed by using Nuclear Magnetic Resonance, Fourier Transform InfraRed (FTIR) spectroscopy and UV Resonant Raman scattering, the origin of some of the spectral contributions having been revealed by proper DFT quantum mechanics simulations. The morphological characterization was done by FTIR imaging and X-ray Computed micro-Tomography.

Our studies demonstrated *nitric* tannin-furanic foams as the nearest approach as an insulating material (e.g., replacement of polystyrene or soft insulation), while *mechanical* tannin-furanic foam is more appropriate as a tough material (e.g., packaging or rigid insulation), bio-based tannin-furanic foams therefore indeed appearing a feasible green alternative to plastic foams derived from fossil fuel-based chemicals.

P18	TUE	COND	14:00 – 15:30	HS 17

How to measure cones of reaction for single-molecule collisions

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At the heart of chemistry is reagents coming together to form products. For this to occur, reagents must collide with one another in the right way. The outcome of the collision depends upon the collision energy (how hard they collide), the relative alignment of reagents (due to steric effects) and on the miss-distance between the centers of mass of the colliding species (termed the impact parameter). It has been shown that the impact parameter can be chosen for on-surface reactions with a "surface-molecular-beam" of a CF_2 “projectiles” [1-2]. This beam is formed by dissociating chemisorbed CF_3 molecules on a Cu(110) surface with a Scanning Tunneling Microscope (STM) tip, with the projectiles being directed along the underlying rows of Cu-atoms toward a chemisorbed molecular target [1-3].

However, in these prior studies the relative alignments of the reagents before the collision was not controlled. This is addressed here through the choice of a singly-debrominated molecular target (DBTF) [4], which can adopt multiple possible adsorption alignments relative to the incoming CF_2 projectile. This allows collision at a selected distance from, and alignment with, the center of mass of the target which is investigated here through experiment and through theoretical calculations of the barriers to reaction for the different target alignments. Thus, this study demonstrates an unprecedented ability to map how collision geometry contributes to collision outcome.

[1] K. Anggara, L. Leung, M. J. Timm, Z. Hu, J. C. Polanyi. Sci Adv. 4, eaau2821 (2018).
[2] K. Anggara, L. Leung, M. J. Timm, Z. Hu, J. C. Polanyi. Faraday Discuss. 214, 89-103 (2019).
[3] M. J. Timm, L. Leung, J. C. Polanyi, J. Am. Chem. Soc. 143, 12644-12649 (2021).
[4] D. Civita, M. Kolmer, G. J. Simpson, A.-P. Li, S. Hecht, L. Grill. Science 370, 957-960 (2020).

P19	TUE	ENS	14:00 – 15:30	HS 17

Procedure of Failure Analysis on Commercial Available Thermoelectric Generator Modules

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In this work, the procedure of failure analysis on commercial available thermoelectric generator modules (TEG) is presented. TEG had been demonstrated to be a promising technique that can convert any form of waste heat directly into the higher-value electrical energy. They are solid-state devices that use the Seebeck effect, with the advantages of having no moving parts, no working fluids, low maintenance costs, easy scalability, noiseless operation and a long life-span. To bring TEG from laboratory status to industrial applications, it is very important that their intrinsic positive properties can be fully exploited through a high long-term stability / reliability.

In order to quantify reliability, defective TEG must be analyzed for their failure mode and failure cause / failure location using non destructive (NDE) and destructive evaluation (DE) techniques. Therefore failure analysis is an important task to determine the root cause of a failure. In this context, it is helpful to make a rough distinction between failure types such as "weak" and "hard" failures.

Weak failure means that the TEG is working, but is out of specification, generally resulting in an increased internal resistance e.g. due to degeneration in the interconnection soldering / TE leg. Hard failure means that the TEG is completely inoperable, i. e. no current can flow due to e. g. internal cracks, defective soldering, broken leg, etc. The applicability of the NDE methods such as measuring the internal resistance as a function of temperature, IR-thermography (hot-spot detection), scanning acoustic microscopy (C-SAM) and X-ray computed tomography is presented.

After performing NDE, DE methods are applied such as embedding the TEG, cutting, grinding and polishing together with optical microscopy, SEM, chemical element analysis such as EDS to determine the location and cause of the defect (root cause of the failure).

P20	TUE	FAKT	14:00 – 15:30	HS 17

CRAB: A novel approach to the calibration of cryogenic particle detectors

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Cryogenic particle detectors (e.g. $CaWO_4$ and Al_2O_3) have found widespread usage in many current experiments, including the investigation of coherent elastic neutrino-nucleus scattering and the search for dark matter candidates. Despite their common deployment as state-of-the-art particle detectors for interactions in the low energy region of about 100 eV, there is currently no feasible method for their calibration in this energy regime.

The CRAB experiment (**C**alibrated **R**ecoils for **A**ccurate **B**olometry) aims to provide a novel approach to the calibration of cryogenic particle detectors in the 100 eV energy regime via nuclear recoils triggered by thermal neutron capture induced gamma emission. The method is based on the thermal neutron capture of a target crystal's nucleus, resulting in its excitation to an unstable energy state. In order to return to a stable, lower energy state, the nucleus emits energy in the form of photons -- either as a single gamma transition or a multi gamma cascade -- which leads to the recoil of the nucleus with an energy of around 100 eV. The recoil energy deposited in the target crystal results in a temperature increase that can be measured using a transition edge sensor. By comparing the calculated recoil energy with the measured spectrum, the cryogenic detector can be calibrated.

Following a successful proof of concept in the form of the publication of a first observation of a nuclear recoil peak in the 100 eV region using the CRAB method, the collaboration's next step is the setup of the experiment at the TRIGA Mk II research reactor at TU Wien in 2024. The experiment's second phase aims to perform a high statistics, low background measurement run improving the precision of the method and providing a reliable calibration for a cryogenic detector crystal.

P21	TUE	FAKT	14:00 – 15:30	HS 17

GRASIAN: Analyses of time of flight distribution of deuterium Beam

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Measurements have shown that neutrons can be trapped between the potential of the earth's gravitational field and the potential of a mirror. This led to the observation of gravitational quantum states (GQS). GQS have not been shown for atoms yet. The aim of the GRAISIAN collaboration is to prove the existence of GQS for atoms. A cryogenic beam source is employed as the methodological approach in this study. This choice is driven by the expectation of achieving higher densities with hydrogen or deuterium relative to neutrons. The investigation of physics beyond the Standard Model, especially hypothetical short-range interactions, could be enhanced due to the expected higher statistics. Therefore, the atoms have to be decelerated to a velocity of $v < 100$ m/s. The velocity distribution for deuterium beam was examined. It could be shown that a velocity range of 73-97 m/s can be resolved.

P22	TUE	FAKT	14:00 – 15:30	HS 17

An ion spectrometer for the identification of molecular bound states with positronium

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In this poster I will show a design for an ion spectrometer with a resolution of 1 amu to explore the formation of molecules with a positronium (Ps) atom. The experiment is located at the positron beam line of the Positron Group of Stefan Meyer Institute of the Austrian Academy of Science.

Starting from a Sodium-22 source, fast positrons are cooled, decelerated and trapped, and are directed to a gas target located inside the spectrometer where they ionize various gases such as methane, water, CO_2 and more to form bound states e.g. PsH, PsO. Ions are extracted from the spectrometer onto a multichannel plate detector (MCP) and their time of flight (ToF) recorded.

Due to the short lifetime of Ps-molecule bound states (~500ps) we cannot observe them directly. By measuring the time of flight of the ions we can determine the binding energies of the PsA (B_{PsA}) by observing the appearance threshold energy of the reaction path e.g.

$e^+ + CH_4 = CH_3^+ + Ps + H$ has E_{thresh}

$e^+ + CH_4 = CH_3^+ + PsH$ has $E_{thresh} - B_{PsH}$

The objective is to measure Time-of-Flight spectra of ions and compare their appearance energy with theoretical calculations, specifically aiming to determine the binding energy of PsA for the various gas species used. Understanding the binding energies of those Positronium Hybrids (PsA) is useful for applications in polymers, semiconductors, thin films, quantum dots, and astrophysics.

By designing a spectrometer with a resolution of 1 amu, utilizing the trap to produce pulses with reduced energy spreads (50 meV) we aim to perform precision measurements on these exotic matter-antimatter bound states.

P23	TUE	MBU	14:00 – 15:30	HS 17

Bottom-up Molecular Control of Biomimetic Hydrogels

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The development of biomimetic hydrogels has greatly facilitated fundamental studies aimed at understanding cellular mechanosensing and mechanotransduction processes. It is now widely accepted that cells sense the elastic and viscoelastic properties of their surroundings and respond to these properties via a range of different mechanisms. It is still unknown, however, how cells determine these material properties. Hydrogels are usually characterized as bulk samples while cells interact with these materials in a highly localized manner via specific receptor-ligand interactions. It is thus essential to adopt the cellular point of view and establish a link between microscopic and macroscopic material properties. Towards this goal, we utilize biomimetic hydrogels consisting of mechanically characterized synthetic polymers and extracellular matrix-inspired peptides that serve as physical crosslinks. Using selected examples, we show how crosslink thermodynamics, kinetics and mechanics as well as network topology affect the linear and non-linear viscoelastic properties of molecularly programmed hydrogels. In particular, we highlight that both individual crosslink properties and network topology affect network stress relaxation and show how molecular bond rupture correlates with bulk material failure. Our modular hydrogel system allows for tuning different parameters independently and thus serves as an excellent platform for disentangling the roles of different material properties on cellular responses.

P24	TUE	MBU	14:00 – 15:30	HS 17

Viscoelastic cell properties from AFM stress relaxation experiments

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This study focuses on the viscoelastic nature of cells, in particular HeLa cells, and their mechanical response to stress. Using atomic force microscopy (AFM), different forces and dwell times were applied to the cells to observe their stress relaxation behaviour. Three linear viscoelasticity models were tested: the standard linear solid model, the five element Maxwell model and the power law model. The experimental results favoured the five element Maxwell model as the most accurate to describe the stress relaxation response of the cells. In addition, the study used self-organising maps (SOMs) to analyse and present the viscoelastic parameters in a compact, two-dimensional format to facilitate interpretation of the data. This research serves as a guide for conducting stress relaxation experiments on soft matter using AFM.

P25	TUE	MBU	14:00 – 15:30	HS 17

Understanding Biodegradation of Polyethylene Terephthalate (PET): a Biophysical Approach

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The surge in global plastic production over the past five decades has reached staggering levels. In 2016, it has approached 335 million metric tons annually, with Europe contributing 60 million metric tons. In response to this, the development of recycling techniques is crucial. While mechanical recycling may compromise plastic quality, and chemical recycling introduces new economic and environmental challenges, biodegradation presents a promising alternative. Within the last ten years, a number of polyethylene terephthalate (PET) degrading enzymes have been found in Nature, such as the PET hydrolase from *Ideonella sakaiensis* 201-F6 (PETase). While a number of studies have confirmed the ability of PETase to degrade bulk PET, our understanding of its interaction with amorphous and crystalline regions remains limited. This work aims to shed light on the molecular process of PET degradation, using an array of experimental and theoretical methods. We have prepared and characterized PET surfaces that expose both amorphous and crystalline regions, as shown with polarization microscopy and atomic force microscopy (AFM). AFM was also used to determine the local activity of wildtype and mutant PETase on these different regions. These degradation experiments are complemented with molecular dynamics simulations to shed light on active site structure and dynamics during PET degradation. Preliminary findings suggest that amorphous PET is degraded faster than crystalline regions. However, at this moment, the stability of the enzyme restricts long-term experiments and further optimization of PETase enzymes is necessary.

P26	TUE	OGD	14:00 – 15:30	HS 17

Gradient-based optimization in tensor LEED

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LEED-*I(V)* extends low-energy electron diffraction (LEED) by measuring the intensity *I* of diffraction beams against the incident electron energy (or, equivalently, the acceleration voltage *V*). These *I(V)* curves provide extensive quantitative insights into the surface structure of the sample. However, due to the absence of phase data in the diffraction measurement, a direct inversion of the *I(V)* curves to a surface structure is impossible. Instead, a guess for a promising surface structure must be made, followed by the computation of *I(V)* curves and their subsequent comparison with experimental data.

The new Vienna package for Erlangen LEED (ViPErLEED) [1] is based on the Erlangen tensor-LEED package (TensErLEED) [2]. TensErLEED employs the perturbative tensor-LEED approximation [3] to accelerate the sampling process during structure optimization. This approach involves conducting the computationally intensive full-dynamic calculation (i.e., including multiple-scattering effects) for a reference surface. Perturbation theory is then utilized to assess the impact of small changes to the reference structure on the resulting amplitudes and intensities. Calculating the amplitude change resulting from these surface modifications is significantly faster than performing a full-dynamic calculation.

The current implementation for calculating amplitude changes and structure optimization was originally devised for relatively simple systems, but it scales poorly when confronted with larger and more challenging structures. To enable efficient calculations for complex surfaces we investigate new algorithms and approaches, such as automatic differentiation, for structure optimization in the established tensor-LEED approach. The translation of the Fortran code to Python enables the utilisation of advanced optimizers available in the Python ecosystem.

[1] F. Kraushofer, A. M. Imre, T. Kißlinger, G. Franceschi, M. Schmid, U. Diebold, L. Hammer, and M. Riva, ViPErLEED package I: Calculation of *I(V)* curves and structural optimization. To be published.
[2] V. Blum and K. Heinz. Fast LEED intensity calculations for surface crystallography using tensor LEED. *Comput. Phys*. *Commun*. **134**, 392 (2001).
[3] P.J. Rous and J.B. Pendry. The theory of tensor LEED. *Surf*. *Sci*. **219**, 355 (1989).

P27	TUE	OGD	14:00 – 15:30	HS 17

Spinel $MgAl_2O_4$(001) reconstruction formed at elevated temperatures

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Resolving the atomic-scale surface structure of spinel oxides is key to understanding the properties of this important class of materials used in heterogeneous catalysis. However, due to their insulating nature, it is experimentally challenging. Noncontact atomic force microscopy (nc-AFM) with a qPlus sensor [1] and well-defined CuOx tip [2] allow us to resolve the surface structure with atomic resolution and chemical sensitivity.

Magnesium aluminate ($MgAl_2O_4$) represents the class of cubic spinels. The polar (001) termination of $MgAl_2O_4$ has been found to form a corrugated surface with elongated protruding ridges at annealing temperatures below 1050 °C [3]. At higher annealing temperatures (1100 °C), the formation of magnesium-aluminum inversions was proposed, and argued to contribute to the polarity compensation [4].

Here, we show that the (001) surface adopts a c(2×4) reconstruction at high annealing temperatures (> 1200 °C), accompanied by a change of the Mg/Al ratio detected by X-ray photoelectron spectroscopy (XPS). We resolve with nc-AFM the surface structure changes induced by increasing annealing temperatures, and the polarity compensation mechanism is discussed.

References:

[1] F. J. Giessibl. *Rev. Sci. Instrum.*, 2019, **90**, 011101

[2] B. Schulze Lammers et al. *Nanoscale*, 2021, **13**, 13617

[3] T. N. Jensen et al. *Phys. Chem. Chem. Phys.*, 2015, **17**, 5795

[4] M. K. Rasmussen et al. *Phys. Rev. B,* 2011, **84**, 235419

P28	TUE	OGD	14:00 – 15:30	HS 17

Surface charges on Ferrolelectrics studied by AFM

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The electric field above polar domains of ferroelectrics are usually diminished by compensating charges. Part of those charges are present in form of ions adsorbed from the ambient [1]. Here, an attempt is made to remove the compensation charges from Lithiumniobate and Bariumtitanate surfaces in order to restore the pristine surface electric field above the ferroelectric domains. In a first step, mechanical removal was tried to accomplish by scanning an atomic force microscopy (AFM) tip in contact mode across the surface. The results were evaluated by electrostatic force microscopy (EFM) [2] and Kelvin probe force microscopy (KPFM) [3] measurements. An additional approach is to desorb the screening species upon heating of the ferroelectrics up to 300°C. Depending on the environmental conditions the restored electric field vanishes with time as indicated by a loss of contrast in EFM signal. This is attributed to readsorbtion of charged species from the ambient. Further investigations aim at the use of the electric field above ferroelectric domains as permanent gates for two-dimensional material based devices.

[1] M.J. Highland et al. Phys. Rev. Lett. 107, 187602 (2011).
[2] B.D. Terris et al. Phys. Rev. Lett 63, 2669 (1989).
[3] M. Nonnenmacher et al. Appl. Phys. Lett. 58, 2921 (1991).

P29	TUE	OGD	14:00 – 15:30	HS 17

Increased Curie temperature and magnetoresistive response by modifying Fe/Mo ratio in Sr_2FeMoO_6 thin films

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We investigated the effect of deposition distance on a set of otherwise identically grown Sr_2FeMoO_6 (SFMO) thin films grown by pulsed laser deposition. Based on the detailed magnetic and transport measurements, we found that the optimal properties can be realized at longer deposition distances than earlier expected. The achieved onset Curie temperature of the order of 400 K with a middle transition value of 372 K, which is clearly the highest presented in the literature for the SFMO thin films. In addition, the increased metallicity and magnetoresistive response is observed in films deposited at longer distances. The improvements are widely discussed in light of the discovered stoichiometric imbalance between the cations Fe and Mo, which modify the magnetic interactions and thus magnetic and electric properties. Therefore, this study shows a new approach in the deposition process to provide multilayers of high quality SFMO thin films for future spin valve devices working at room temperature.

The optimization of SFMO thin films depends on several parameters, and target-to-substrate distance is one of the important parameter. For example, the deposition distance has been demonstrated to influence the stoichiometric balance of the material. This provides a clear variable for further deposition optimization and understanding about the effects of off-stoichiometry in SFMO thin films. In our system, we have used the deposition distance (3.2 cm) for the fabrication of smoother thin films and achieved high crystallinity. Therefore, the main objective of this work is to find the optimal deposition distance for obtaining as high as possible T_C and magnetoresistive response in the SFMO thin films, by fixing the optimized deposition temperature and atmosphere. We have addressed the effect of deposition distance and structural characteristics of the films on magnetic and magneto-transport properties. Based on the experimental results, the orientations for achieving optimal SFMO films for future applications are proposed [1].

1. Naushahi, N. A., Angervo, I., Saloaro, M., Schulman, A., Huhtinen, H., & Paturi, P. (2022). Increased Curie temperature and magnetoresistive response by modifying Fe/Mo ratio in Sr_2FeMoO_6 thin films. Journal of Magnetism and Magnetic Materials, 564, 169990.

P30	TUE	OGD	14:00 – 15:30	HS 17

Growth of (Si)Ge nanosheets by MBE at ultra-low temperatures for nanoelectronics applications

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In recent decades, heteroepitaxial layers comprising crystalline stacks of Group-IV alloys, predominantly SiGe, have been employed to enhance the operational efficiency of Si-based devices [1]. However, achieving defect-free pseudomorphic (Si)Ge layers on Si(001) substrates with high Ge compositions ($x \gtrsim 50\%$) poses significant challenges due to strain-induced relaxation beyond a layer thickness of a few monolayers [2].

This study explores molecular beam epitaxy (MBE) growth at ultra-low temperatures (ULT), ranging from 100°C to 350°C, departing from conventional epitaxy temperatures (>500°C). Reduced surface kinetics in ULT conditions leads to notable layer supersaturation, allowing for the growth of thicker pseudomorphic layers than previously achieved [3]. We show that maintaining pristine growth pressures at the lower end of the ultra-high-vacuum range (~10^{-11} mbar) is crucial to minimizing impurities and preserving superior electrical and optical properties of grown heterostructures. This is particularly true during ULT growth, where a limited thermal budget hampers efficient gas desorption from substrates.

Here, we demonstrate that the combination of ULT and excellent growth pressures enables the fabrication of high-quality thin films, exemplified by fully strained, defect-free (Si)Ge epitaxial layers directly grown on Si and silicon-on-insulator (SOI) substrates. These layers exhibit remarkable structural qualities, as confirmed by Atomic Force Microscopy (AFM), X-ray diffraction (XRD) and transmission electron microscopy (TEM) experiments [3]. Furthermore, we show that these nanosheets serve as a scalable platform for advanced SiGe and Ge-based reconfigurable field-effect transistors, capable of dynamic run-time switching between n- and p-type operation, exhibiting outstanding performance [4], [5]. For these devices, high-resolution TEM reveals sharp and reproducible interfaces with single-element crystalline Al contacts formed through a thermally induced Al-Si1-xGex exchange reaction [6]. The precisely chosen (Si)Ge channel stoichiometry and abrupt interfaces contribute to exceptional symmetric I-V operability in RFET devices, as observed in their transfer characteristics[4], [5].

[1] I. A. Fischer *et al.*, *APL Photonic*s, **2022**, vol. 7, no. 5, p. 050901.
[2] M. Brehm and M. Grydlik, *Nanotechnology*, **2017**, vol. 28, no. 39, p. 392001.
[3] A. Salomon *et al*., *Phys. Status solidi*, **2022**, vol. 219, no. 17, p. 2200154.
[4] A. Fuchsberger *et al., Adv. Electron Mater.*, **2023**, vol. 9, no. 6, p. 2201259.
[5] A. Fuchsberger *et al., IEEE J. Electron Devices Soc*., **2024**, vol. 18, no. 9, pp. 83-87.
[6] L. Wind *et al.*, *Small*, **2022**, vol. 18, no. 44, p. 2204178.

P31	TUE	OGD	14:00 – 15:30	HS 17

Group IV double-heterostructure light-emitting diodes operating at room temperature

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For integrating optoelectronic components such as light-emitting diodes (LEDs) or lasers into existing CMOS-based technology, it would be of great advantage if the components could be processed using Si technology. However, Si and Ge are intrinsically poor light emitters due to their indirect band gap, and Ge/Si heterostructures are of type-II band alignment, i.e., charge carrier separation further hinders light emission.

Here, we show that double-heterostructures (DHS) LEDs made from Si/SiGe/Si layer stacks emit light at telecom wavelengths and room temperature and above. However, such room temperature operation is only possible if the SiGe layer thickness is far higher than conventional experimental limits for layer relaxation. The samples were grown in an MBE system on a n-doped Si-substrate followed by a n-doped Si buffer-layer, the p-n-junction is formed by a n-doped and a p-doped SiGe layer with a sufficiently high layer thickness (≥ 16 nm) to avoid quantum confinement and finally capped by a final p-doped Si layer. The growth at a very low pressure of ≤ 10^{-10} mbar and at ultra-low temperature of ~300°C is an essential prerequisite for a defect-free, pseudomorphic growth of sufficiently thick $Si_{0.6}Ge_{0.4}$ layers (≥ 16 nm) on a Si buffer layer [1]. Transmission electron microscope (TEM) measurements and obtained device parameters confirm a perfect lattice quality attributed to the aforementioned growth parameters.

The main benefit of this newly developed group-IV DHS is the conversion from type-II to type-I band offsets for higher applied bias voltage [2,3]. Consequently, electroluminescence measurements of our $Si/Si_{0.6}Ge_{0.4}/Si$ DHS samples show a high emission rate at telecom wavelengths, adjustable by the Ge content. Adding quantum dots to form a dot-in-well heterostructure stabilizes the emission intensity and the spectral position of the emitted light from low temperatures (10 K) up to 360 K, which corresponds to the maximum available sample temperature without relevant thermal quenching [3].

Furthermore, device simulations suggest that the DHS structures can have a high internal quantum efficiency. As a first step towards reducing the losses, we addressed current crowding by making design adjustments. Additionally, we were able to improve the line width and temperature stability by embedding quantum dots [3].

Thus, we present the first successful demonstration of these group-IV and type-I electrically-pumped double heterostructure light sources that emit in the telecom wavelength range and can be operated from low temperatures up to room temperature and beyond.

[1] A. Salomon *et al.*, Phys. Status. Solidi A., doi:10.1002/pssa.202200154 (2022)
[2] Patent in preparation.
[3] A. Salomon *et al.*, in preparation

P32	TUE	OGD	14:00 – 15:30	HS 17

Searching for new polymorphs by epitaxial growth

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The formation of unknown polymorphs due to the crystallization at a substrate surface is frequently observed. This phenomenon is much less studied for epitaxially grown molecular crystals, since the unambiguous proof of a new polymorph is a challenging task. The existence of multiple epitaxial alignments of the crystallites together with the simultaneous presence of different polymorphs do not allow simple phase identification.

We present grazing incidence X-ray diffraction (GIXD) studies with sample rotation on epitaxially grown film (with thicknesses from 10 to 30 nm) on conjugated molecules like PTCDA, 6,13-pentacenequinone (P2O), 1,2;8,9-dibenzopentacene (trans-DBPen) and dicyanovinyl-quaterthiophene (DCV4T-Et2) grown by physical vapour deposition on Ag(111) and Cu(111) single crystals. A new method for indexing the observed Bragg peaks allows the determination of the crystallographic unit cells so that the type of crystallographic phase can be clearly identified. This approach even works when several polymorphs are simultaneously present within a single sample as shown for DCV4T-Et2 on Ag(111). Additionally, epitaxial relationships between the epitaxially grown crystallites and the single crystalline surfaces are determined.

The origin of new polymorphs is due to nucleation on single crystal surfaces. The first monolayer is only accessible by surface sensitive methods that allow the determination of a two-dimensional lattice like low-energy electron diffraction (LEED). Therefore, we compare our results on the three-dimensional lattice with LEED experiments on molecular monolayers of the same conjugated molecules. A correlation between the first monolayer and the epitaxial growth of three-dimensional crystals together with lattice distortions and re-alignment of molecules can be observed. The selected examples show three possible scenarios of crystal growth on top of an ordered monolayer: (i) growth of a single polymorph, (ii) growth of three different polymorphs; in both cases the first monolayer serves as template. In the third case (iii) strong lattice distortion and distinct molecular re-alignments from the monolayer to epitaxially grown crystals are found.

P33	TUE	OGD	14:00 – 15:30	HS 17

Calibrated Microwave Reflectance Microscopy in a Scanning Tunnelling Microscope

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Technological innovation relies on the ability of scientists to discover, understand and harness the power of phenomena nature has to offer. Development of smaller, faster and more complex technologies requires techniques that characterise materials and devices with spatial resolutions down to the single atom scale.

The microwave frequency range (0.3 to 300 GHz) is the domain of many high-potential phenomena, including magnetic resonances, collective spin and electron mode resonances, and dipolar relaxation. Despite the importance of the GHz frequency range, microwave characterisation and spectroscopy of materials at the nanoscale has proven to be a significant challenge. This has potentially hampered the adoption of promising material systems, such as charge density wave materials or skyrmions, for practical applications.

In order to bridge the gap between bulk microwave spectroscopy and the nanoscale, we have implemented microwave reflection microscopy in an ultra-high vacuum cryogenic scanning tunnelling microscope. We present the experimental set-up, along with preliminary data demonstrating the sensitivity and spatial resolution of our microwave reflection measurements. We will show our recently developed in-situ calibration procedure, which enables quantitative measurement of the frequency dependent impedance at the tunnelling junction. This enables the characterisation of important material properties, including conductivity, relative dielectric permittivity, and doping concentrations, of nanoscale functional materials and devices. These results open the door to microwave impedance spectroscopic fingerprinting down to the scale of single molecules.

P34	TUE	OGD	14:00 – 15:30	HS 17

A new system for ferroelectric Rashba semiconductors based on Ge-doped PbSe

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Ferroelectric Rashba semiconductors (FERSC) exhibiting a giant Rashba splitting are a new class of multifunctional materials that are highly promising for spintronic devices. Although vast variety of materials have been theoretically predicted as FERSC, the experimental realization is still limited to a few compounds, such as GeTe[1], SnTe[2], and $Pb_{1-x}Ge_xTe$[3], that, however, exhibit a high intrinsic p-type conductivity that is detrimental for device applications. In this work, a new material system for FERSC is presented based on Germanium doped PbSe. This way, a high-quality ternary ferroelectric $Pb_{1-x}Ge_xSe$ alloy with large ferroelectric Rashba effect in the ferroelectric phase is formed. $Pb_{1-x}Ge_xSe$ epilayers were grown by molecular beam epitaxy using PbSe and GeSe sources. Due to the high vapor pressure of GeSe, low temperature growth is required to achieve a significant Ge incorporation. Despite the remarkably low-temperature growth window of $Pb_{1-x}Ge_xSe$, the epilayers display high quality pseudomorphic layer-by-layer 2D growth and atomically smooth surfaces with the monoatomic steps. Ge incorporation induces a ferroelectric lattice distortion of cubic PbSe below a critical T_C that strongly increases with the Ge content up to values around 200 K for x_{Ge} = 8%. This is signified by the resistivity anomaly in $Pb_{1-x}Ge_xSe$ films observed at T_C. The effect of ferroelectricity on the electronic band structure was determined by angle resolved photoemission spectroscopy performed at the URANOS beamline of the SOLARIS synchrotron facility. For thin $Pb_{1-x}Ge_xSe$ quantum wells, we observe a strong momentum Rashba splitting of the quantized subbands emerging in the ferroelectric phase below the T_C that is absent in the cubic phase. The magnitude of the splitting is temperature-dependent and increases with higher Ge concentration, which clearly proves $Pb_{1-x}Ge_xSe$ as a FERSC. Thus, a high-quality ternary ferroelectric $Pb_{1-x}Ge_xSe$ alloy produced by low-temperature epitaxy is experimentally demonstrated as a new alternative compound semiconductor for FERSC.

[1] G. Kremer, J. Maklar, L. Nicolaï, et al. *Nat. Commun.* **13**, 6396 (2022).
[2] F. Chassot, A. Pulkkinen, G. Kremer, T. Zakusylo, et al. *Nano Letters* **24** (1), 82 (2024).
[3] G. Krizman, T. Zakusylo, L. Sajeev, M. Hajlaoui, et al. *Adv. Mater.* **23**, 2310278 (2023).

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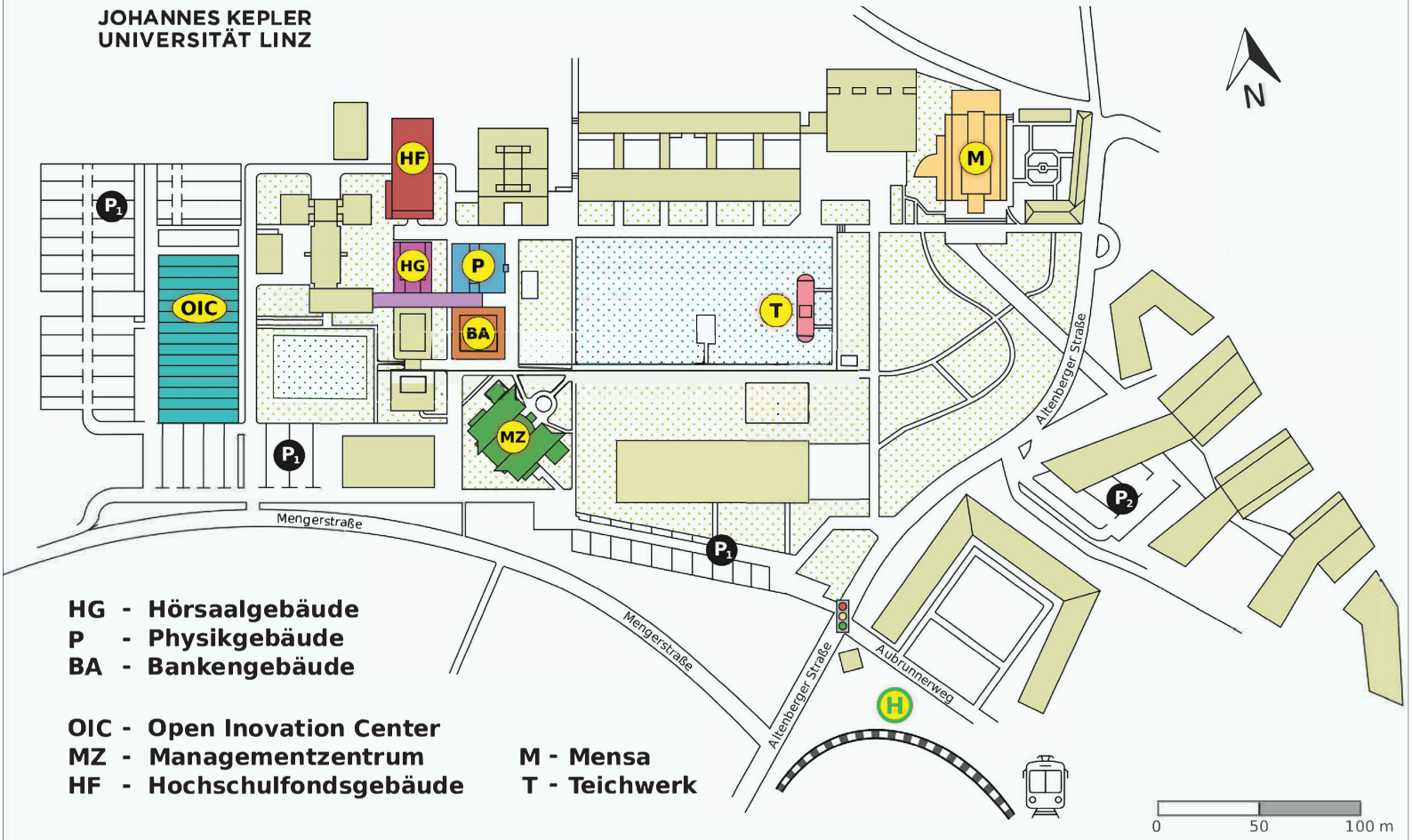

HG - Hörsaalgebäude
P - Physikgebäude
BA - Bankengebäude

OIC - Open Inovation Center
MZ - Managementzentrum
HF - Hochschulfondsgebäude

M - Mensa
T - Teichwerk