



68th Annual Meeting of the Austrian Physical Society

September 10th - 13th, 2018

Institute of Experimental Physics, Graz University of Technology



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of the Austrian Physical Society

Program
& Abstracts

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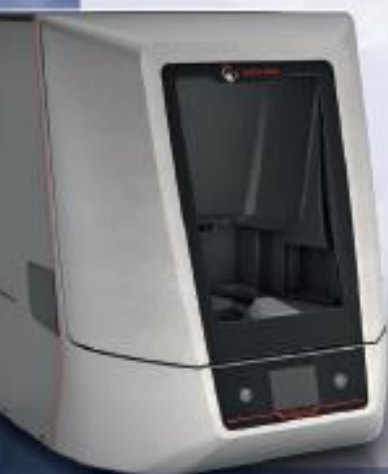


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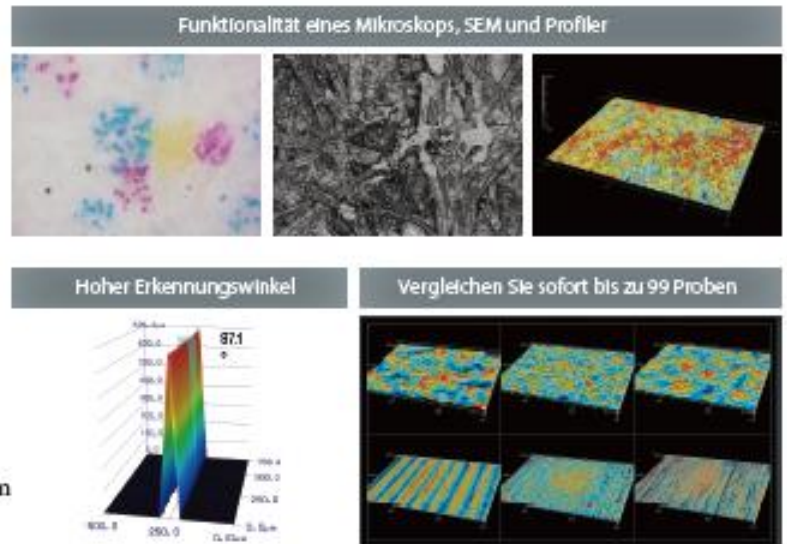
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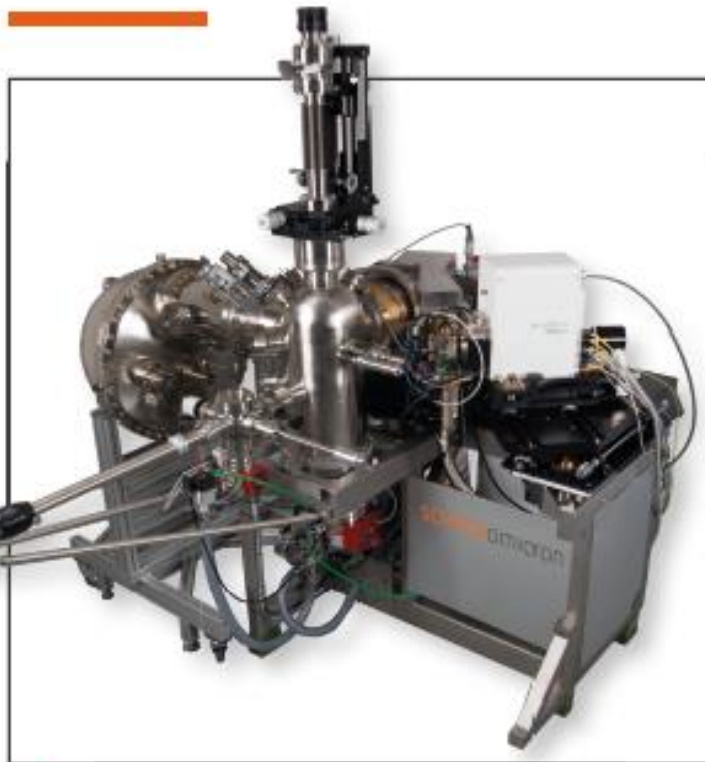


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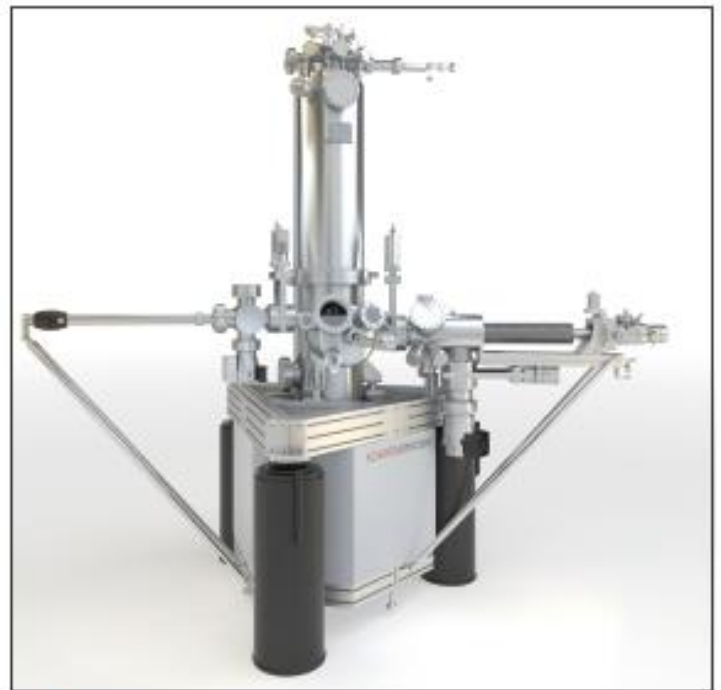
A window to the bulk



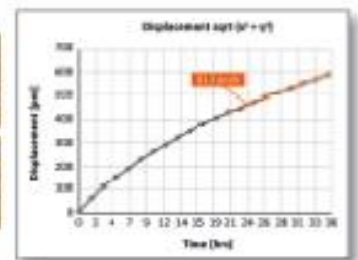
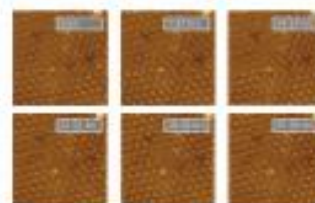
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Contents

Introduction	5
Local Organisation	6
Organizers	6
Local Organisation Committee	6
Conference Information	7
Conference Site and Location of Lecture Halls	7
Registration / Information Desk	8
Conference Fees, Payment	9
Internet Access	9
Lecture Rooms	9
Oral Presentation	9
Poster Presentation	10
Coffee Breaks	10
Nearby Restaurants	10
Reception by Mayor of the City of Graz	10
Time Schedule	11
Plenary Speakers	14
Evening Lecture	18
Awards	19
Fritz Kohlrausch Prize	19
Roman Sexl Prize	20
Max Auwärter Prize	20
Technical Meetings of Divisions	22
Acoustics (AKU)	22
Atoms, Molecules, Quantum Optics and Plasmas (AMP)	24
Condensed Matter (COND)	33
Extreme Light Infrastructure (ELI)	50
Nuclear and Particle Physics (FAKT)	56
History of Physics (GEP)	66
Physics and School (LHS)	70
Medical Physics, Biophysics and Environmental Physics (MBU)	72
Surfaces, Interfaces and Thin Layers (OGD)	77
Physics-Industry (PIN)	98
Poster Contributions of Divisions	101
Atoms, Molecules, Quantum Optics and Plasmas (AMP)	101
Condensed Matter (COND)	105
Nuclear and Particle Physics (FAKT)	111
Medical Physics, Biophysics and Environmental Physics (MBU)	114
Research with Neutron and Synchrotron Radiation (NESY)	115
Surfaces, Interfaces and Thin Layers (OGD)	116
Physics-Industry (PIN)	135
Exhibitors	137

Sponsors	138
LIST OF AUTHORS	140

Introduction

The 68th Annual Meeting of the Austrian Physical Society is organized by the Institute of Experimental Physics at Graz University of Technology, Austria, and will take place in the Physics Building, with the postal address Petersgasse 16, 8010 Graz.

The purpose of this conference is to promote physics in Austria, disseminate the results of physics research, and bring Austrian physicists together to exchange their views.

Seven plenary lectures and one public evening lecture will be given by internationally renowned experts.

Recent research results in the following areas will be covered in several oral sessions within the conference: Acoustics; Atoms, Molecules, Quantum Optics and Plasmas; Condensed Matter; Extreme Light Infrastructure; Nuclear and Particle Physics; History of Physics; Physics and School; Medical Physics; Biophysics and Environmental Physics; Research with Neutron and Synchrotron Radiation; Surfaces, Interfaces and Thin Layers; Physics-Industry and Polymer Physics. In addition, poster presentations are planned for all the above named topics.

The following Prizes of the Austrian Physical Society will be awarded this year:

1. The Fritz Kohlrausch Prize which is biennially awarded to a young experimental investigator for excellent research, alternating with the Ludwig Boltzmann Prize for theoretical physics every other year.
2. The Roman Ulrich Sexl Prize which is awarded for exceptional services in teaching physics at school and university. The awardees are selected in close cooperation with the Division "Physics and School".
3. The Student Prize of the Austrian Physical Society is awarded for outstanding master's or diploma theses in the fields of experimental or theoretical physics, in close cooperation with the Working Group "Young Minds".
4. The Division "Physics and School" also selects exceptional candidates from schools to present them special awards for their "pre-scientific work".
5. The Division "Surfaces, Interfaces, and Thin Films" presents the Max Auwärter Prize, an award for "outstanding achievements in the physics of surfaces and boundary layers".

Organisation Committee

Organizers

Prof. Wolfgang E. Ernst	Institute of Experimental Physics, Graz University of Technology wolfgang.ernst@tugraz.at, +43 (0) 316 / 873 - 8140
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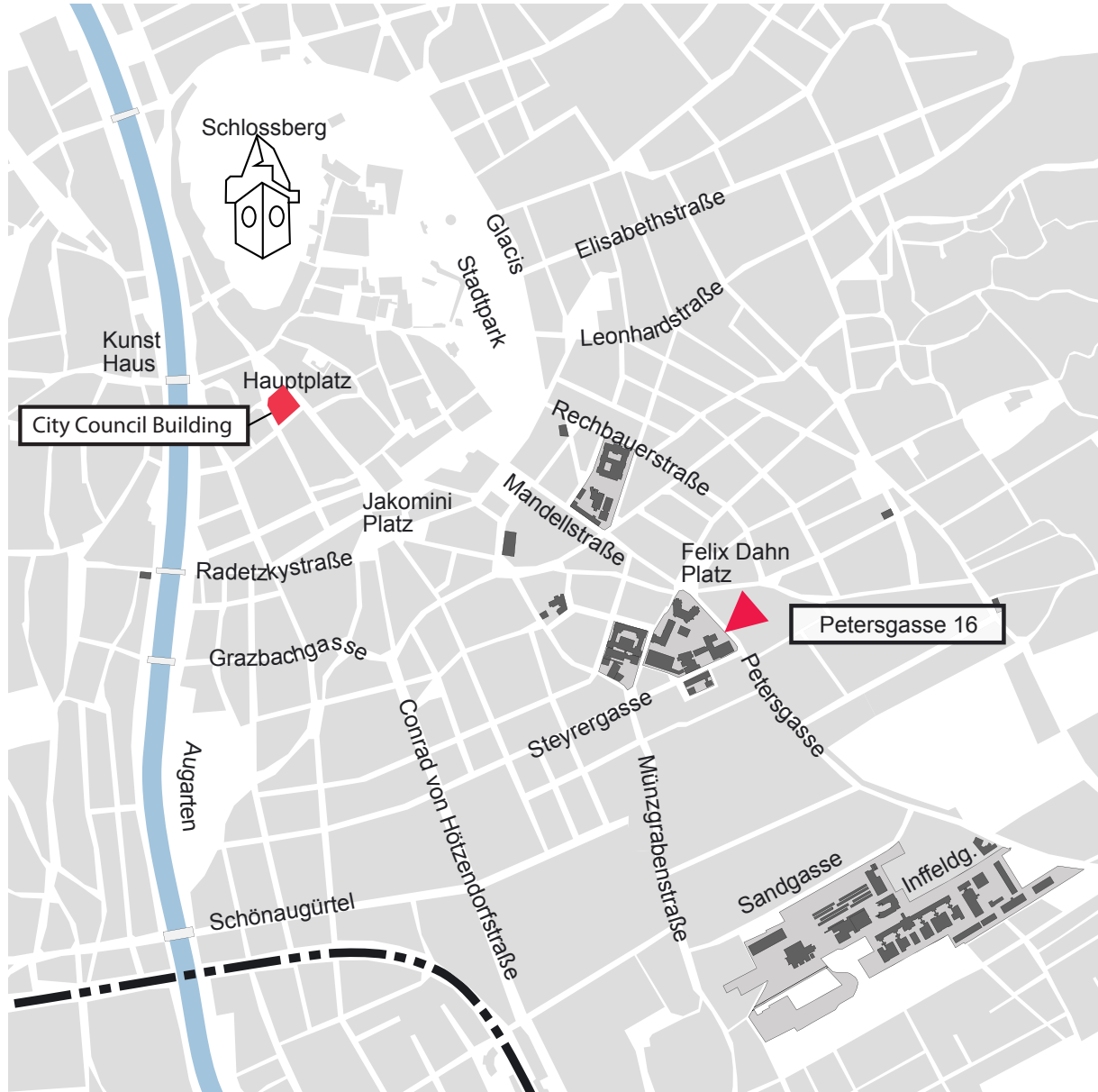
The local organisation is performed by members of the Institute of Experimental Physics at Graz University of Technology.

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Conference Information¹

Conference Site and Location of Lecture Halls

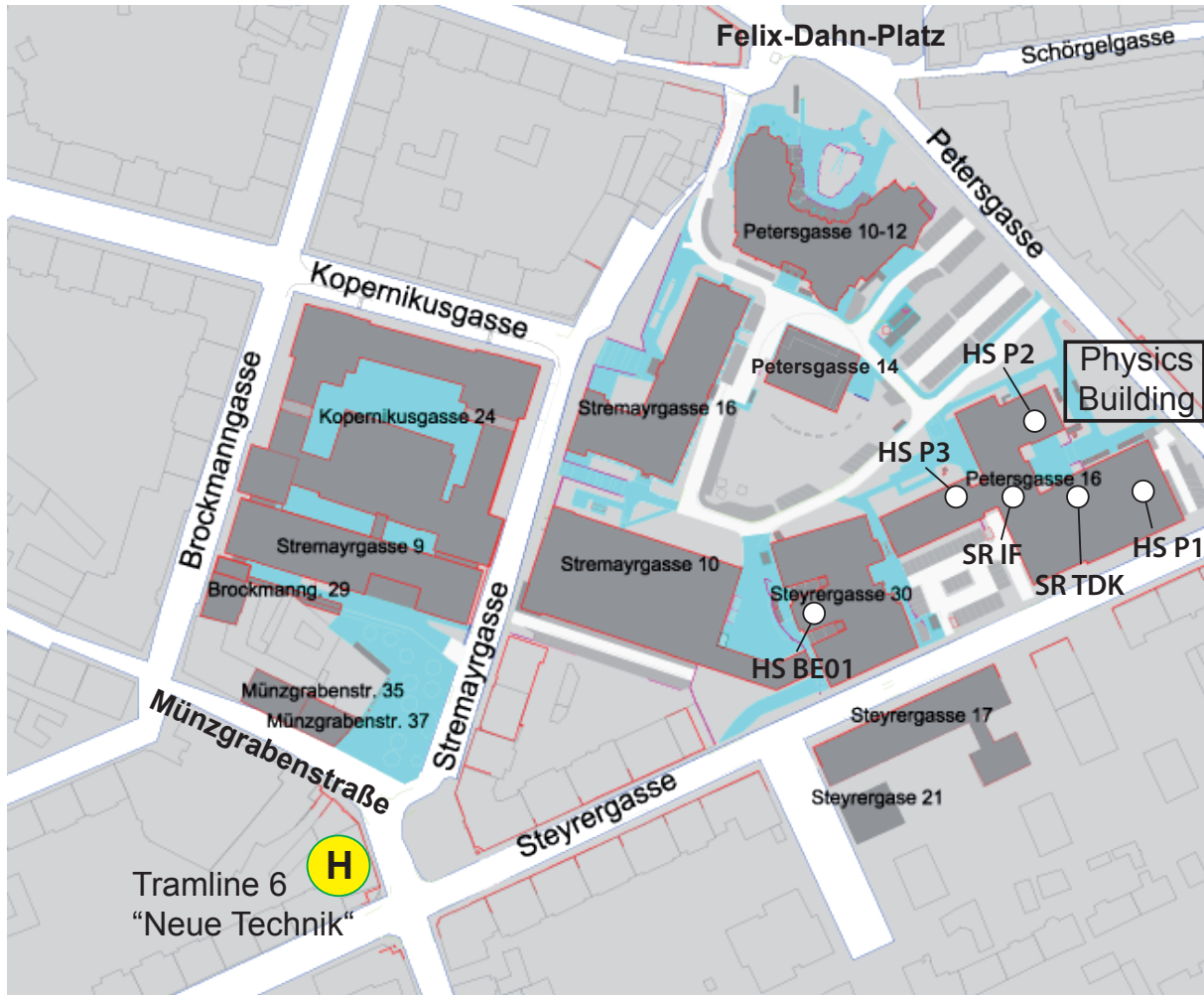


Part of a map of Graz, indicating the conference site at the Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria ("Physics Building", GPS coordinates: 47.064709 N, 15.454195 E.) and the City Council Building at Hauptplatz where a reception by the Mayor of the City of Graz will be given on Tuesday, Sep 11, 19:00.

The conference will take place at the Institute of Experimental Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria ("Physics Building"). Lecture halls in the physics building as well as next door at Steyrergasse 30 will be used for the conference. The participants of the conference are

¹More detailed informations and relevant links, as well as photographs and graphical illustrations you can find on the conference homepage <https://www.tugraz.at/events/oepg-2018/home/>.

encouraged to use public transportation. The tram stop "Neue Technik" of tramline 6 is suggested to be used, especially if you arrive/depart at the Graz main railway station (direct connection using this tramline). The parking area is limited, you can park your car in blue zones around the conference site up to 3 hours. Next parking garages are within 15 minutes walking distance.



The locations of the lecture halls used for the conference on the TU campus "Neue Technik" are indicated by white dots.

Designation	Room Code	Address/Entrance
HS P1	PHEG024C	Petersgasse 16 (entrance 1st floor)
HS P2	PHEG002	Petersgasse 16 (groundfloor)
HS P3	PH02112	Petersgasse 16 (2nd floor)
SR TDK	PHEG016	Petersgasse 16 (groundfloor)
HS BE01	STEG140	Steyrergasse 30 (groundfloor)
SR IF	PH01150	Petersgasse 16 (1st floor)

Registration / Information Desk

The registration desk is located on the ground floor and is to be accessed through the entrance to the Institute of Experimental Physics. The conference office is open from Tuesday to Thursday (September 11th - 13th) from 8 - 12, on Tuesday also from 13 - 16. Outside these hours, help by the conference team is available at the administrative office of the institute opposite the registration desk.

All participants please report at the registration desk before visiting any session. You will receive your name badge, conference program and further documents. For all activities please have your nametag well visible with you!

Conference Fees, Payment

Members	100,-
Non-members	130,-
PhD Student members	80,-
PhD Student non-members	100,-
Students before master	60,-

Registration fees include:

- The program and abstract booklet and the usual conference giveaways
- Access to all plenary and regular sessions
- All coffee breaks
- Refreshments during the poster sessions

We kindly ask you to pay the conference fee in advance. This way you shorten the waiting time at the registration desk, facilitate our work and even save money!

Payments should be made to:

Technische Universität Graz
UniCredit Bank Austria
Herrengasse 15, 8010 Graz
IBAN: AT211200010013630768
BIC: BKAUATWW

Reference (Verwendungszweck): Invoice Number + participant's names!

A late fee of €20,- will be applied for registrations after July 31st.

After your successful registration you will get an invoice via e-mail within a few days. After receipt of payment you will receive a confirmation of payment if you mark it during your registration. At the registration desk you can only pay cash (EUR). We unfortunately do not accept any credit cards.

Attention: Fees are not refundable in the event of cancellation!

Internet Access

During the conference WLAN access is available for all participants. Login data will be received with registration. The EDUROAM network is also installed at Graz University of Technology.

Equipment of Lecture Rooms

All rooms are equipped with beamers, blackboards and a PC.

Oral Presentation

Please arrive at your session 15 minutes before the session starts to set up your presentation on the local computer and to introduce yourself to the session chairperson. We request that you have your presentation stored on a USB-stick which you will use to upload your presentation to our local computer in the lecture hall. As we have a very tight schedule, please make sure to keep your time. You can find the allotted time of your talk in the book of abstracts.

Poster Presentation

The Poster Session will take place in the afternoons of Tuesday and Wednesday in the basement of the physics building. The poster boards are numbered according to the program, so every participant will find their board easily. All posters are expected to be on display on the assigned days. **The poster format has to be A1 (594 mm wide × 841 mm height)**. Material to fix your poster like adhesive tape or pins will be provided by the organizers. We kindly ask the presenters to stay close to their respective posters during the poster sessions.

Coffee Breaks

The coffee breaks will take place on the first floor in front of lecture hall HS P1. The conference fee will cover coffee breaks and the refreshments during the poster sessions. The restaurants in the nearby city are at your disposal for lunch.

Nearby Restaurants

For informations on daily menus for lunch at some restaurants around Graz University of Technology please look at the corresponding topics of the conference homepage.

<https://www.tugraz.at/events/oepg-2018/home/>.

There you can also receive information about restaurants offering vegetarian and vegan menus.

Reception by Mayor of the City of Graz

A reception by the Mayor of the City of Graz will be given on Tuesday, Sep 11 at 19:00 in the City Council Building at Hauptplatz 1, 8010 Graz. All tramlines stop at Hauptplatz.

Time Schedule

A full-week timetable you can find on the back cover of the book of abstracts!

Monday, September 10

13:00-17:30	Energy Day	HS P1
17:30-18:00	—	
18:00-19:15	ÖPG Board Meeting	SR IF

Tuesday, September 11

08:00-12:00	REGISTRATION	
13:00-16:00	REGISTRATION	
09:00-09:30	Opening	HS P1
09:30-10:15	Plenary Talk-1: Gottfried Strasser	HS P1
10:15-10:30	COFFEE	
10:30-11:15	Plenary Talk-2: Markus Arndt	HS P1
11:15-12:00	Plenary Talk-3: Peter Heering	HS P1
12:00-14:00	LUNCH BREAK	
14:00-15:30	Technical Meetings of Divisions	
	COND Session I	14:00-15:30 HS P2
	GEP Session I	14:00-15:20 SR TDK
	OGD Session I	14:00-15:30 HS BE01
15:30-16:00	COFFEE	
16:00-17:30	Technical Meetings of Divisions	
	AKU Session I	16:00-17:00 HS P3
	COND Session II	16:00-17:30 HS P2
	GEP Session II	16:00-17:20 SR TDK
	OGD Session II	16:00-17:30 HS BE01
17:30-18:30	Poster Session	Basement
18:30-19:00	—	
19:00-20:00	Reception by Mayor of the City of Graz	City Council Building

Wednesday, September 12

08:00-12:00	REGISTRATION		
09:00-09:45	Plenary Talk-4: Hans-Peter Steinrück		HS P1
09:45-10:30	Plenary Talk-5: Michela Mapelli		HS P1
10:30-10:45	COFFEE		
10:45-12:00	Prize Award Celebration Session		HS P1
12:00-13:00	LUNCH BREAK		
13:00-14:00	General Assembly of ÖPG Members		HS P1
14:00-15:30	Technical Meetings of Divisions		
	COND Session III	14:00-15:30	HS P2
	ELI Session I	14:00-15-30	SR IF
	FAKT Session I	14:00-15:30	SR TDK
	LHS and YM Session I	14:00-15:30	HS P1
	PIN Session I	14:00-15:20	HS P3
	OGD Session III	14:00-15:30	HS BE01
15:30-16:00	COFFEE		
16:00-17:30	Technical Meetings of Divisions		
	AMP Session I	16:00-17:20	HS P3
	COND Sess. IV + NESY Sess. I	16:00-17:30	HS P2
	ELI Session II	16:00-17:10	SR IF
	FAKT Session II	16:00-17:30	SR TDK
	LHS and YM Session II	16:00-17:30	HS P1
	OGD Session IV	16:00-17:30	HS BE01
17:30-19:00	Poster Session		Basement
19:00-20:30	Evening Lecture: Prof. Ferenc Krausz (with reception)		HS P1

Thursday, September 13

08:00-12:00	REGISTRATION		
09:00-09:45	Plenary Talk-6: Horst Hahn		HS P1
09:45-10:30	Plenary Talk-7: Federica Petricca		HS P1
10:30-10:45	COFFEE		
10:45-11:15	Kohlrausch Prize Talk		HS P1
11:15-11:45	Sextl Prize Talk		HS P1
11:45-12:15	Auwärter Prize Talk		HS P1
12:15-14:00	LUNCH BREAK		
14:00-15:30	Technical Meetings of Divisions		
	AMP Session II	14:00-15:30	HS P3
	FAKT Session III	14:00-15:30	SR TDK
	MBU Session I	14:00-15:30	HS P2
	OGD Session V	14:00-15:30	HS BE01
15:30-16:00	COFFEE		
16:00-17:30	Technical Meetings of Divisions		
	AMP Session III	16:00-17:20	HS P3
	FAKT Session IV	16:00-17:35	SR TDK
	OGD Session VI	16:00-17:30	HS BE01
17:30	Closing of the Conference		

List of Acronyms for Divisions and Working Groups of the Austrian Physical Society

ACP	Equal Opportunities in Physics
AKE	Energy
AKU	Acoustics
AMP	Atoms, Molecules, Quantum Optics and Plasmas
COND	Condensed Matter
ELI	Extreme Light Infrastructure
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
PMP	Polymer Physics
YM	Young Minds

Plenary Lectures

PLENARY TALK-1 9:30-10:15 TUESDAY, SEP 11

HS P1

Applied Quantum Mechanics: Sensing with Monolithically Integrated Quantum Cascade Devices

Gottfried Strasser

Institute of Solid State Electronics, Technische Universität Wien, Vienna, Austria

Center for Micro- and Nanostructures, Technische Universität Wien, Vienna, Austria

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This talk aims to give a short introduction in the field of quantum devices with a strong focus on quantum cascade lasers (QCLs) and quantum cascade detectors (QCDs). Since the first proposal using intraband transitions in QWs to achieve lasing (Kazarinov and Suris in the seventies) and their first experimental realization at Bell Laboratories in the nineties intraband and interband cascade lasers have been intensively studied in terms of bandstructure engineering, cavity design and fabrication technology. Nowadays, QC lasers are compact and coherent light sources covering the spectral range from the mid-infrared to the terahertz region.

A bi-functional QC structure will be presented, that can be operated in two modes, as coherent light emitter as well as intraband detector, depending on the bias applied to the structure. Today, photonic devices are widely used in environmental and industrial process control and/or monitoring as well as medical and biochemical diagnostics. Conventional optical sensing setups include a light source, a light-analyte interaction region and a separate detector. We developed and improved a sensor concept based on a bi-functional quantum cascade heterostructure, for which the differentiation between laser and detector is eliminated. Apart from the fascinating physics of light-matter interaction, this enables mutual commutation of laser and detector, simplifies remote sensing setups and allows crucial miniaturization of sensing devices for further integration.

PLENARY TALK-2 10:30-11:15 TUESDAY, SEP 11

HS P1

Probing Quantum Linearity with Biomolecules and High Mass Nanoparticles

Markus Arndt

University of Vienna, Faculty of Physics, QNP Group, VCQ, Boltzmannngasse 5, A-1090 Vienna, Austria

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Quantum physics is our best theory of nature, but important questions have remained: Why is quantum mechanics linear, allowing for superpositions of classically mutually exclusive states that we do not see on the macroscopic scale we live in? What is the role of complexity or gravity in the quantum-to-classical transition? Can we utilize non-classical superpositions for novel measurements?

Starting from text-book like matter-wave diffraction experiments we will analyze which beam splitter and configurations are needed to see de Broglie interference of massive and complex particles in the lab. We see that molecular matter waves can be delocalized in position and momentum, even when each molecule avails of a rich set of internal vibrational, rotational and conformational states with a variety of electronic and optical properties. Quantum coherence in the center of mass motion persists even at internal microcanonical temperatures of 500 - 1000 K. It even was seen for molecules as massive as 10'000 amu and even molecules that we eat every day can be delocalized.

What is it then, that prevents the realization of Schrödinger cat states in our macroscopic world? The search for possible mass and complexity limits of quantum linearity is experimentally valid, independent of any theory. I will discuss the most recent interferometer developments that will allow to push this limit by almost two orders of magnitude and progress in nanoparticle source developments as required and foreseeable to realize matter-wave interference for free-falling particles of $10^7 - 10^8$ amu.

PLENARY TALK-3 11:15-12:00 TUESDAY, SEP 11

HS P1

Analysing historical experiments with the replication method

Peter Heering

*Institut für mathematische, naturwissenschaftliche und technische Bildung
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Experiments have been considered for a long time as central to knowledge production in physics. From this perspective, it may seem remarkable that the historiography of science addressed the practical aspects of experiments only a few decades ago. Yet, since the 1980s, experimental practices as well as material aspects have received more attention.

In the presentation, I will discuss a particular approach towards experimental practices from the past: the replication method which aims at understanding practices through re-enacting these practices. In order to show the potential of this approach, the analysis of some canonical experiments from the history of physics will be discussed. In doing so, the educational potential of these case studies will also be sketched.

PLENARY TALK-4 9:00-9:45 WEDNESDAY, SEP 12

HS P1

Surface science of low-vapor-pressure liquids

Hans-Peter Steinrück

Physical Chemistry, Universität Erlangen-Nürnberg

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Low-vapor-pressure liquids can be investigated using the methods surface science. In particular, angle-resolved XPS provides access to the liquid/gas(vacuum) and liquid/solid interfaces. It even allows for *in situ* studies of chemical reactions in the liquid. We report on recent investigations of ionic liquids¹ and of novel supported liquid metal catalysts.² The experiments were performed with our near-ambient pressure XPS lab setup, and with a newly developed two-analyzer lab-based XPS system that allows for simultaneous measurements of low-viscosity liquids at normal (0°) and grazing emission (80°).³

[1] F. Maier, I. Niedermaier, H.-P. Steinrück, *J. Chem. Phys.* **146** (2017) 170901 1-15

[2] N. Taccardi, M. Grabau, C. Papp, H.-P. Steinrück, P. Wasserscheid, *Nat. Chem.* **9** (2017) 862

[3] I. Niedermaier, C. Kolbeck, H.-P. Steinrück, F. Maier, *Rev. Sci. Instrum.* **87** (2016) 045105 1

The dawn of gravitational wave astrophysics and the formation channels of compact object binaries

Michela Mapelli

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On September 14 2015, the LIGO interferometers captured a gravitational wave (GW) signal from two merging black holes (BHs), opening the era of gravitational wave astronomy. Five BH mergers and one neutron star (NS) merger have been reported so far. Understanding their formation channels is currently one of the main challenges of astrophysics. In this talk, I will discuss the impact of progenitor's metallicity and of several binary evolution processes on the mass of merging compact objects. Dynamical processes also affect the formation of compact object binaries: dynamical exchanges in star clusters can lead to the formation of massive binaries with relatively high eccentricity and misaligned spins. The runaway collision process can even lead to the formation of intermediate-mass black holes. Finally, I will discuss the BH merger rate evolution across cosmic time and the properties of the host galaxies of compact object binaries.

Design of materials properties by microstructure and external fields

Horst Hahn

Institute for Nanotechnology, Karlsruhe Institute of Technology (KIT)
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The mechanical, physical and chemical properties of materials are determined by their microstructure. Modern materials science uses the complex interplay of defects, such as impurities, phases, point and line defects and interfaces, to tailor properties and obtain high-performance metallic alloys and ceramics. In this approach of materials design, properties can only be changed by modifying their microstructure, for example by initiating grain growth during annealing at elevated temperatures. Such a behavior, that fixes the properties irreversibly to the microstructure, is advantageous for many applications of materials, where long-term stability of the properties is required. Recent examples for designing materials properties will be presented, nanoglasses, cluster-deposited glasses and high entropy oxides.

In contrast, tuning using external fields, i.e., electric, offers completely new opportunities for the fully reversible control of materials properties. Such tuning of physical properties will be demonstrated for several nanostructures, i.e. (epitaxial) thin films, nanoporous, nanoparticulate structures and nanowires. Tuning can be either achieved using dielectric/ferroelectric gating, well known from semiconductor physics, or by electrolyte gating using liquid or solid electrolytes. Furthermore, using electrochemical ion intercalation, fully reversible properties with substantially larger effect magnitude can be achieved.

Finally, the concepts employed for tuning properties of nanostructures can be employed in applications as well. As an example, field-effect transistors based on inorganic nanoparticles as the channel material and solid electrolyte for the gating will be described.

Catching dark matter: Status and future of direct detection

Federica Petricca

Max-Planck-Institut für Physik, Werner-Heisenberg-Institut, Föhringer Ring 6, 80805 München, Deutschland

petricca@mpp.mpg.de

The dark matter problem has accompanied cosmologist and particle physicist for more than 80 years. Nowadays we have an extremely accurate model of our Universe, but still most of its content eludes our observation. The observation of this missing matter is of compelling necessity for our understanding. Direct searches aim to detect dark matter particles with Earth-bound detectors. A review of the most sensitive technologies and of recent results is given together with a glance into the perspectives.

Evening Lecture

WEDNESDAY, SEP 12 19:00-20:30

HS P1

Schnellste Vorgänge im Mikrokosmos: Von der Grundlagenforschung bis hin zur Krebsbekämpfung

Ferenc Krausz

Max-Planck-Institut für Quantenoptik, Garching, Deutschland

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In unserem Leben spielen Elektronen eine elementare Rolle. Ihre Bewegungen steuern alle chemischen Prozesse in der Natur. Ebenso bestimmen Elektronen die Geschwindigkeit unserer Computer- und Informationstechnologien. Bewegungen der Elementarteilchen und Lichtwellen bedingen sich gegenseitig, auf der Zeitskala von Attosekunden, also Milliardstel von Milliardstel Sekunden.

Um zu erkunden, was in so kurzen Zeiträumen im Mikrokosmos passiert, benötigt man Lichtblitze, die ebenfalls nur Attosekunden lang dauern. Solche Blitze wurden in der Arbeitsgruppe von Professor Krausz in Wien im Jahr 2001 erstmals produziert. Diese Technologie ermöglicht es nun erstmals, in Echtzeit zu verfolgen, wie sich ultraschnelle Phänomene um die Kerne von Atomen herum abspielen.

In den letzten Jahren sind die Attosekunden-Technologien den Kinderschuhen entwachsen und zu verlässlichen Messtechniken gereift. Jetzt eröffnen sie neue Wege um etwa Krankheiten, wie Krebs, frühzeitig zu detektieren. Die Grundlage dafür bieten Messungen kleinster Veränderungen in der molekularen Zusammensetzung von Blut mittels direkten Abtastens ultraschnell schwingender elektrischer Felder, die durch angeregte Moleküle ausgesendet werden.

Awards

The Price-Awards Celebration Session takes place on Wednesday from 10:45 - 12:00 in lecture hall HS P1. The talks of the prize winners are given on Thursday between 10:45-12:15 in lecture hall HS P1, too.

Fritz Kohlrausch Prize

AWARD-1 10:45-11:15 THURSDAY, SEP 13

HS P1

Controlling Microwave Photons with Micromechanical Oscillators

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Superconducting circuits are at the focus of quantum engineering research because of their potential for scalable quantum information processing. One disadvantage of circuit QED systems is that they can only operate in ultra-cold environments where thermal noise and resistive losses are negligible. To enable larger scale superconducting quantum networks we are working towards an on-chip integrated microwave-photonic device that has the potential to efficiently convert microwave to telecom wavelength photons using radiation pressure forces. Utilizing compact ultra-high impedance LC circuits suspended on dielectric nano-membranes enables efficient coupling to the mechanical modes of one-dimensional nanobeam oscillators compatible with nano-photonics [1]. With our new silicon-on-insulator platform [2] we demonstrate motional ground state cooling, voltage tuneable microwave frequency conversion, superconducting qubit integration [3], the realization of highly nonreciprocal on-chip isolators and circulators [4], and the synthesis of non-classical photon states. Moving to higher frequency acoustic bandgap defined modes should allow to generate mechanical quantum states without the need for active cooling. Coupling to photonic crystals on the other hand would put within reach the realization of hybrid long distance quantum communication networks. We will present our most recent progress towards these long term goals.

[1] J. M. Fink, M. Kalae, A. Pitanti, R. Norte, L. Heinzle, M. Davanço, K. Srinivasan, and O. Painter, “Quantum electromechanics on silicon nitride nanomembranes”, *Nature Communications* **7**, 12396 (2016)

[2] Paul B. Dieterle, Mahmoud Kalae, Johannes M. Fink, and Oskar Painter, “Superconducting Cavity Electromechanics on a Silicon-On-Insulator Platform”, *Physical Review Applied* **6**, 014013 (2016)

[3] Andrew J. Keller, Paul B. Dieterle, Michael Fang, Brett Berger, Johannes M. Fink, Oskar Painter, “Al transmon qubits on silicon-on-insulator for quantum device integration”, *Applied Physics Letters* **111**, 042603 (2017)

[4] S. Barzanjeh, M. Wulf, M. Peruzzo, M. Kalae, P. B. Dieterle, O. Painter, J. M. Fink, “Mechanical On-Chip Microwave Circulator”, *Nature Communications* **9**, 953 (2017)

Roman Sendl Prize

AWARD-2 11:15-11:45 THURSDAY, SEP 13

HS P1

Ausgewählte Experimente zum Thema Levitation

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Der Begriff *Levitation* - von lateinisch *levitas* (Leichtigkeit) - steht für ein technisches Verfahren, bei dem Objekte zum Schweben gebracht werden, weiters für klassische Tricks in der Zauberkunst, aber auch für ein parapsychologisches Phänomen, bei dem Menschen und Gegenstände unerklärlich zu schweben scheinen.

Im Rahmen dieser Experimentiervorlesung werden Beispiele für elektromagnetische Levitation, elektrostatische Levitation, aerodynamische Levitation, akustische Levitation, magnetische/diamagnetische Levitation, sowie Levitation aufgrund des Archimedischen Prinzips vorgeführt. Die Anwendung der jeweiligen Methode in der wissenschaftlichen Forschung wird an Hand von speziellen Experimenten demonstriert und führt uns bis hin zur internationalen Raumstation ISS. Auch der eine oder andere Zaubertrick steht am Programm.

Max Auwärter Prize

AWARD-3 11:45-12:15 THURSDAY, SEP 13

HS P1

Magnetic remanence in single atoms

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Stabilizing the magnetization of a single surface-adsorbed atom is the key to store and process information in the smallest unit of matter. To achieve this goal, it is required to stabilize the spin of the magnetic atom against thermal and quantum fluctuations. For a decade, the research in the field focused on *3d* atoms [1]. However, they all show a paramagnetic behavior down to 0.3 K [2]. Recently, the focus of the research shifted to rare earth atoms, whose *4f* electrons provide large magnetic moments and anisotropies, as well as an efficient decoupling from the environment.

In this talk, I will show that rare earth atoms exhibit magnetic stability on the timescale of hours when adsorbed on ultra-thin decoupling layers grown on a metal substrate. First, we used X-ray magnetic circular dichroism (XMCD) to prove that Ho atoms on MgO/Ag(100) exhibit magnetic stability, with a spin lifetime of 1500 s at 10 K and hysteretic loops up to 40 K [3]. These features qualify them as the first single atom magnets. Second, combining XMCD with scanning tunneling microscopy, we realized a model bit patterned media made of single Dy atoms. When deposited on graphene/Ir(111), these atoms exhibit magnetic stability at 2.5 K. In addition, the moiré pattern originating from the graphene/Ir lattice mismatch drives a self-assembly mechanism, which allows organizing the Dy

atoms into ordered arrays [4]. Our results pave the road to magnetic information storage at the single atom level.

[1] P. Gambardella *et al.*, *Science* **300**, 1130 (2003).

[2] Focko Meier *et al.*, *Science* **320**, 82 (2008); I. G. Rau *et al.*, *Science* **344**, 988 (2014).

[3] E. Donati *et al.*, *Science* **352**, 318 (2016).

[4] R. Baltic *et al.*, *Nano Lett.* **16**, 7610 (2016).

Technical Meetings of Divisions

ACOUSTICS

(AKU)

AKU SESSION I 16:00-17:00 TUESDAY, SEP 11

HS P3

AKU-1 TALK 16:00-16:20 TUESDAY, SEP 11

HS P3

MicLocator - Determining multiple microphones' positions using sound wave delay and trilateration

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This presentation is part of the SilentAirHP project conducted at AIT, which aims at reducing the sound emission of heat pumps. In this framework, an acoustic dome with 64 microphones is used to capture frequency-, time-, and space resolved acoustic data. In order to efficiently determine the position of these microphones, i.e. their spatial coordinates, an ultrasonic solution using trilateration has been developed. Six speakers have been placed in 3D-space and their coordinates have been measured manually. Recording a specific sound sample played back on each of the speakers with predetermined time delay, the algorithm correlates the sound source data with that of the sound receiver, i.e. the microphone. After converting the resulting soundwave travel times to distances, the trilateration algorithm can be applied, which uses Newton's approximation to solve the spherical equations expressing the travel distance of the sound wave from each speaker to the microphone. The obtained coordinates enable the validation of the geometry of the 64 microphones used in the acoustic dome and the calculation of the representative area of each microphone for later sound power evaluation and 3D visualization. In the long run, an optimized calculation could be used for Augmented Reality and (slow) motion capturing. The work consisted of building a prototype solution, making it compatible to the other systems in use, preparing the hardware and developing a full GUI software solution. SilentAirHP is supported in the framework of the Energy research program of the Climate and Energy Fund (5148527) initiated by the Austrian Ministry for Transport, Innovation and Technology.

Determining the Influence of the Operating Point on Noise Emissions of Air Source Heat Pumps

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The role of heat pumps for space heating is becoming more and more significant in Austria and Europe. Especially in single-family detached homes, the air source heat pump is becoming a standard heating system. Since the heat source is outside air, it is typical for such a device to make use of an outside heat exchanger unit. This will cause noise emissions, which have to be accounted for in acoustic planning, e.g., calculating the required minimum distance of the outside unit to sensitive areas like bedroom windows. The noise emission specifications on these devices represent a state of standard operation. Other operating points, most notably the defrosting of the heat exchanger, can be significantly louder. The main goal is to examine the noise emissions of an air source heat pump at different points of operation. This is done inside a conventional acoustics test facility. Since such a facility does not offer the simulation of outside air, fan heaters and ultrasonic humidifiers are used to ensure constant temperature and humidity levels.

The paper presents spectra and sound power levels at standard operation points which are currently used for the declared sound power level. Additionally the sound power levels and spectra over time during typical operation phases are presented and discussed.

Gaussian Closure für hysteretische Systeme unter weißem Rauschen

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Für nichtlineare Systeme unter weißer Rausch-Anregung stellt die Gaussian Closure eine gute Approximation dar. Es wird der spezielle Fall der von Bouc beschriebenen Hysterese vorgestellt. Dabei kann mit der Gaussian Closure sowohl der stationäre als auch der transiente Vorgang behandelt werden. Hier wird nur der transiente Fall vorgestellt. In diesem Fall ist es nicht erforderlich, eine elastische Rückstellkraft zusätzlich zur hysteretischen Kraft anzunehmen. Daneben ist es möglich, auch Exzentrizitäten der Belastung, zeitliche Veränderlichkeit der Belastungen und Parameter und gefiltertes weißes Rauschen zu behandeln. Ebenso können auch Mehrfreiheitsgradprobleme behandelt werden. Allerdings steigt der Rechenaufwand rasch mit der Anzahl der Freiheitsgrade an. Auch werden bei Mehrfreiheitsgradproblemen Probleme in der Stabilität der Gleichungen beobachtet.

ATOMS, MOLECULES, QUANTUM OPTICS and PLASMAS

(AMP)

AMP SESSION I 16:00-17:20 WEDNESDAY, SEP 12

HS P3

AMP-1 TALK 16:00-16:20 WEDNESDAY, SEP 12

HS P3

A coupled dark state magnetometer developed for space missions

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The development of an optically pumped magnetometer for space missions is a challenging task considering the electrical, mechanical and thermal limitations and restrictions in a harsh environment. The coupled dark state magnetometer (CDSM) is a self-calibrating, scalar magnetometer specifically designed for these challenges [1].

The coherent population trapping effect (CPT), within the hyper fine structure of the ⁸⁷Rb – D₁ line, allows a precise detection of magnetic fields. Several of these CPT resonances, in the form of Λ -systems, are excited and coupled simultaneously to minimize external influences such as neon buffer gas pressure shift, vapor cell temperature shift and light shift. Depending on the angle between the magnetic field and the laser propagation axis the resonances are switched to enable an omnidirectional sensitivity to magnetic fields [2].

The CDSM's current space ready flight model features a compact and robust design. Optical fibres connect the ⁸⁷Rb sensor unit to a vertical cavity surface emitting laser (VCSEL) diode unit and a photodiode, both within an electronics unit. This unit's footprint measures 24.0 x 18.0 cm. The laser light is FM-modulated with a 3.4 GHz signal to match the ground state splitting of the Λ -systems. A field programmable gate array (FPGA) ensures the autonomous operation in space. The fully operational CDSM consumes less than 4 W of electric power. Currently an absolute accuracy below 0.5 nT is achieved.

Since February of 2018, the first CDSM version has been operating successfully in a low earth orbit as part of the china seismo-electromagnetic satellite (CSES) mission. In 2022 a further developed version will be launched on board of the Jupiter icy moons explorer (JUICE) mission. An overview of the device and recent developments will be presented.

[1] R. Lammegger, *WIPO*, Patent WO/2008/151344 (2008).

[2] A. Pollinger, M. Ellmeier, W. Magnes, C. Hagen, W. Baumjohann, E. Leitgeb and R. Lammegger, *IEEE Instr. and Meas. Technology Conference (I2MTC) Proceedings*, **33** (2012)

Super- and subradiance of a 1D chain of clock atoms trapped inside an optical fiber

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Atoms resonantly coupled to the transversely confined propagating field modes of a optical nanofiber will exchange energy via virtually infinite range fiber mediated and free space dipole dipole interaction. For a sufficiently large number of emitters regularly arranged in a magic wavelength lattice, fiber interaction dominates free space coupling and emission. We predict drastic modifications of the atomic decay and shifts of the emission frequency. We study the example of superradiant forward decay from the fully inverted state including free space emission and coupling to transverse fiber modes of a hollow core fiber. Using various levels of approximation starting from a solution of the full master equation to different orders of mean field expansions we study systems from a few to experimentally relevantly many particles.

The influence of spacetime curvature on quantum emission in optical analogues to gravity

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Quantum vacuum fluctuations on curved spacetimes cause the emission of entangled pairs. The most remarkable instance of this effect is Hawking radiation from black hole horizons, which can however not be observed in astrophysics. Fortunately, it is possible to recreate the kinematics of waves on curved spacetimes in the laboratory to study spontaneous emission from the vacuum. Here we investigate the influence of the spacetime curvature, i.e., when there is a horizon or not, on this effect. We develop a field theoretical description based on an optical analogue system to calculate the scattering matrix that completely describes mode coupling leading to the emission of photons in various curvature configurations. We find that horizons lead to an order of magnitude increase in the emission strength, a characteristic shape of the emission spectrum, and a simplification and increase of the quantum spectral correlations. Thus, we demonstrate the role of laboratory horizons for the production of entangled pairs. The findings clarify a number of open questions towards the detection of the Hawking effect in optical and non-optical systems exhibiting horizons.

Bayesian Analysis of Femtosecond Pump-Probe Photoelectron-Photoion Coincidence Measurements

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Ultrafast processes in photoexcited molecules in gas phase are usually investigated by pump-probe photoionization studies, in which transient photoelectron kinetic energies and/or ion masses are recorded. The signals give insight into underlying relaxation processes, but if photoexcited molecules dissociate or multiple species are present, the photoelectron spectra of different species are superimposed, which limits the reliability of certain interpretations. Applying photoelectron-photoion coincidence (PEPICO) detection allows to disentangle these different channels and gives therefore additional insight into the molecular species at the moment of ionization. However, due to detection efficiencies less than unity, coincidence measurements are recorded at low ionization rates in order to reduce the influence of so called false coincidences, where the detected electron-ion pair stems not from the same ionization event and therefore distorts the measured spectra. This leads to long data acquisition times so that this powerful tool often cannot be applied, especially if one is limited to low repetition-rate light sources.

Here we present a probabilistic approach based on Bayesian probability theory to reduce data acquisition times drastically and improve the overall quality of the spectra by directly and consistently estimating the underlying spectra [1]. This approach enables us to (i) increase the signal-to-noise ratio, (ii) subtract background signals (which is a challenging task in coincidence measurements), (iii) exclude false coincidences from the spectra, (iv) include prior information such as positivity of the spectra, (v) compute confidence intervals and (vi) apply it to any experimental situation and noise statistics. We tested our method with challenging mock data and apply it to measured coincidence spectra of acetone molecules, enabling us to estimate fragmentation ratios, which was previously not possible due to unknown contributions of false coincidences.

[1] Rumetshofer, M., Heim, P., Thaler, B., Ernst, W. E., Koch, M., & von der Linden, W. (2017). "Analysis of femtosecond pump-probe photoelectron-photoion coincidence measurements applying Bayesian probability theory". *arXiv preprint arXiv:1709.04456*.

AMP-5 TALK 14:00-14:20 THURSDAY, SEP 13

HS P3

Ramsey set-up for (anti-)hydrogen hyperfine spectroscopy

Amit Nanda on behalf of the ASACUSA collaboration

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In the framework of the Standard Model, CPT symmetry demands the same fundamental properties for matter and antimatter. The precise measurement of the ground state hyperfine structure of antihydrogen and its comparison to that of hydrogen is a sensitive test of CPT invariance. This motivates the ASACUSA (Atomic Spectroscopy And Collisions Using Slow Antiprotons) collaboration based at the Antiproton Decelerator at CERN to measure the ground state hyperfine structure of antihydrogen, and it aims for a ppm level relative precision with a Rabi-type beam experiment [1,2]. ASACUSA produces antihydrogen atoms by the mixing of antiprotons with positrons in a double cusp trap with strong magnetic field gradients for the formation of a polarised beam [5].

For the Rabi-type experiment, a spectrometer line with a strip-line microwave cavity has been fully commissioned with studies on hydrogen. With the use of this spectroscopy apparatus a relative precision of 10^{-9} has been achieved, which is so far the most precise measurement of the hyperfine splitting of hydrogen in beam experiment [3]. A Ramsey type beam spectroscopy method has the potential to improve this precision by a factor of 10 and the implementation of this technique is the topic of my PhD thesis. However, the existing device for driving the hyperfine transitions, namely a strip line cavity, is not well suited for the Ramsey scheme. This called for the design of new microwave devices.

I will present the status of the ASACUSA antihydrogen program [4] with a focus on the recent results on hydrogen and a discussion on the options available for microwave devices in a Ramsey setup, which have been studied with finite element simulations. Although the characterisation of the Ramsey spectrometer line will be done using hydrogen, its scalability for the case of antihydrogen has to be considered as well.

[1] A. Mohri and Y. Yamazaki, *Europhys. Lett.* **63**, 207-213 (2003).

[2] E. Widmann et al., *Hyperfine Interact.* **215**, 1-8 (2013).

[3] M. Diermaier et al., *Nat. Commun.* **8**, 15749 (2017).

[4] C. Malbrunot et al., *Philosophical Transactions of the Royal Society A* **376**, 2116 (2018).

[5] Kuroda, N. et al. *Nat. Commun.* **5**, 3089 (2014).

AMP-6 TALK 14:20-14:40 THURSDAY, SEP 13

HS P3

Neural network based embedded atom model potentials for metallic nanoparticles

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Molecular dynamics simulations of large systems are only feasible if paired with a computationally inexpensive method of calculating the corresponding electronic potential energy surface. Therefore,

a construction of reliable, yet simple interatomic potentials from *ab initio* data is a necessity for dynamic simulations. Standard approaches can be divided into two groups: One is based on physically motivated expressions for energy contributions such as stretching, bending, torsion, and undirected interactions. The other group employs purely mathematically inspired potential forms, which are kept as general as possible in order to resemble any given PES shape in principle. This group of approaches is where machine learning algorithms are typically applied, most notably in an atomic neural network setup as has been suggested by Behler and Parinello. [1]

Atomic neural networks allow for an accurate interpolation of the training data but often fail at the generalization to other systems and lack physically correct asymptotic behavior. On the other hand, physically motivated potentials based on the embedded atom model, such as the Gupta potential [2], often fail to reproduce *ab initio* data due to their limited flexibility. It is our aim to bridge this gap by modeling the physically derived ingredients of the embedded atom model approach via neural networks. This way, we incorporate additional, physical information, which improves the generalization but also ensures a correct behavior in regions of the potential energy surface where *ab initio* data points are rare.

[1] J. Behler and M. Parinello, “Generalized Neural-Network Representation of High-Dimensional Potential-Energy Surfaces”, *Phys. Rev. Lett.* **98**, 146401, 2007.

[2] R. P. Gupta, “Lattice relaxation at a metal surface”, *Phys. Rev. B* **23**, 6265, 1981

AMP-7 TALK 14:40-14:55 THURSDAY, SEP 13

HS P3

Atomic diffraction through a pristine sheet of single layer graphene

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In many applications, the sensitivity of matter-wave interferometers to external perturbations scales with the area enclosed by the delocalized quantum particle. Complementary to the international trend of reaching for the slowest possible particle and longest interaction time, we here explore the feasibility of ultra-wide-angle beam splitting in the extreme opposite parameter range of fast atomic hydrogen. The interaction of H-atoms at 80 eV with single layer graphene was studied using molecular dynamics simulations, based on time-dependent density functional theory. Despite sizable coupling of the atom to the electronic system of graphene, we find a high probability for coherent diffraction through about a sixth of every hexagon in the carbon lattice.

The natural lattice period of only 246 pm yields very large diffraction angles between 10-50 mrad even for hydrogen traveling at 120 000 m/s. Since gravitational free fall is almost negligible on a laboratory scale one can conceive of very large atom interferometer areas in the future. They shall enable new studies in nanoscale material science, force sensing, matter-wave metrology and new tests on the foundations of physics.

Selecting molecular conformers by matter-wave diffraction

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Molecular conformations are of utmost importance in molecular recognition processes and recent collision studies have demonstrated the strong influence of molecular conformation on bimolecular reaction rates [1]. It is therefore of great interest to develop methods that are capable of separating single structures even from a congested conformational space. Here propose a new method that can separate conformers independently of their molecular dipole moment or spin state [2]. By diffraction the matter-wave at a near-resonant ultraviolet optical grating, individual conformers of complex molecules can be spatially isolated in a selected diffraction order. We illustrate the principle and discuss how to prepare a conformer-pure molecular beam of the neurotransmitter 2-phenylethylamine. The technique thus paves the way for structure-sensitive experiments with hydrocarbons and biomolecules, such as neurotransmitters and hormones, which evaded conformer-pure isolation so far. The applications range from environmental research, biomolecular physics to astrophysics.

[1] Y.-P. Chang, K. Długołęcki, J. Küpper, D. Rösch, D. Wild, and S. Willitsch, *Science* **342**, 98 (2013)

[2] C. Brand, B. A. Stickler, C. Knobloch, A. Shayeghi, K. Hornberger, and M. Arndt, *ArXiv* 1710.01035 (2017)

Non-Adiabatic Photofragmentation Dynamics of Acetone Molecules Studied by Femtosecond Photoelectron-Photoion Coincidence Spectroscopy

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For the investigation of photochemical processes with time-resolved photoionization spectroscopy, it is essential to obtain unequivocal experimental information about the fragmentation dynamics. Photoexcitation of acetone molecules to high-lying Rydberg states triggers complex relaxation dynamics which are governed by Rydberg-valence couplings. We apply time-resolved photoelectron-photoion coincidence (PEPICO) detection to disentangle parallel ionization channels and to follow the fragmentation and relaxation behavior of each channel separately [1]. Photoexcited population undergoes internal conversion to lower Rydberg states for which a sequential decay model reveals state-dependent decay time constants ranging from 100 to 300 fs, revealing a monotonic relation between time constant and state energy [2]. The corresponding non-adiabatic dynamics cause the conversion of electronic to vibrational energy, leading to fragmentation after ionization to the cationic ground state, for which the activation threshold can be accurately determined to be (0.79 ± 0.04) eV [3]. The influence of molecular symmetry on electronic relaxation via internal conversion was investigated for low lying Rydberg states (3p), where a coupling between the 3p substates can be directly observed. A newly developed method based on Bayesian probability theory

was applied for data analysis to improve the quality of the measured spectra [4].

Our results demonstrate that in the complex situation of multiple, parallel relaxation pathways, information obtained with PEPICO detection is essential for unambiguous interpretation of transient signals.

[1] P. Maierhofer, M. Bainschab, B. Thaler, P. Heim, W. E. Ernst, and M. Koch, *J Phys. Chem. A* **120**, 6418 (2016).

[2] M. Koch, B. Thaler, P. Heim, and W. E. Ernst, *J. Phys. Chem. A* **121**, 6398 (2017)

[3] M. Koch, P. Heim, B. Thaler, M. Kitzler, and W. E. Ernst, *J. Phys. B* **50**, 125102 (2017)

[4] M. Rumetshofer, P. Heim, B. Thaler, W.E. Ernst, M. Koch, and W. von der Linden, accepted by *Phys. Rev. A* (2018), *arXiv:1709.04456*

AMP SESSION III 16:00-17:20 THURSDAY, SEP 13

HS P3

AMP-10 TALK 16:00-16:20 THURSDAY, SEP 13

HS P3

Ultrafast photoexcitation dynamics inside superfluid helium nanodroplets

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Superfluid helium nanodroplets (He_N) are a widely used tool for spectroscopic investigations of isolated atoms, molecules and clusters at 0.37 K temperature. As they can be loaded with virtually any species, they are a promising approach for time-resolved studies of previously inaccessible systems like weakly-bound clusters, tailor-made molecules or microsolvation environments.

Here we present the very first step towards femtochemistry inside He_N by applying time-resolved photoelectron and photoion spectroscopy to atoms immersed in the quantum fluid. Photoexcitation of single indium atoms, which are confined in a solvation shell bubble inside the droplet, leads to an expansion and oscillation of this bubble accompanied by ejection of the atoms out of the droplet [1]. These pronounced photoexcitation dynamics can be understood in terms of repulsive interactions between the radially extended electron density of the excited atomic state and the closed-shell helium. We follow the transient processes by observing changes in photoelectron kinetic energies, which are a sensitive probe to study the dopant-bath environment, and support the interpretation of our results with time dependent helium-density-functional-theory (TDHeDFT) simulations. In combination, the full energetics of the dynamics is deduced and a mechanistic picture of the influence of the quantum fluid on ultrafast dynamics can be drawn. The corresponding time scales range from a few hundred femtoseconds to several picoseconds, setting the benchmark for the investigation of ultrafast processes that can be accessed inside the droplets.

[1] B. Thaler, S. Ranftl, P. Heim, S. Cesnik, L. Treiber, R. Meyer, A. W. Hauser, W. E. Ernst, M. Koch, in review, *arXiv:1804.04497* (2018)

Coherent vibrational wave packet motion inside superfluid helium nanodroplets

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Superfluid helium nanodroplets (He_N), which have been routinely used for decades to synthesize weakly bound molecules, represent a novel sample preparation technique to study ultrafast dynamics in previously inaccessible systems. Here we present first time-resolved investigations of molecules located inside He_N , obtained with femtosecond pump-probe spectroscopy and photoelectron/photoion probing.

Photoexcitation of indium dimer (In_2) molecules, which are confined in a solvation shell bubble inside He_N , leads to the creation of coherent vibrational wave packet motion in an electronically excited state. As for In atoms [1], photoexcitation leads also to expansion of the helium solvation shell within the first picosecond after excitation, followed by the ejection of the molecules within about 60 ps. For the In_2 we show that during the ejection process no vibrational energy seems to be dissipated to the helium surrounding. We observe for the first time pronounced wave packet dynamics for a molecule fully immersed inside the He_N , as well as the appearance of fractional and full revivals after ejection from the droplet. Our findings show that, surprisingly, coherence is at least partially conserved during the rather strong interaction of the dopant molecule with its helium surrounding. This demonstrates the feasibility of femtochemistry experiments inside He_N , paving the way for further investigation of more complex coherent molecular dynamics.

[1] B. Thaler, S. Ranftl, P. Heim, S. Cesnik, L. Treiber, R. Meyer, A. W. Hauser, W. E. Ernst, M. Koch, in review, *arXiv:1804.04497* (2018)

Subradiance in V-type Multi Level Systems

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Spontaneous emission in quantum emitters can be modified by other emitters nearby, leading to super- and subradiance. We demonstrate the subradiant behaviour of V-type multilevel emitters in close vicinity to each other, with specific examples being an equilateral triangle and a linear chain at interatomic distances below the transition wavelength. For the equivalent triangle an analytical treatment is possible for a very symmetric configuration. In this setup the Hamiltonian features a maximally entangled, antisymmetric eigenstate involving superpositions of all three atoms which exhibits subradiance as opposed to superradiance. Moreover, it decouples completely from the vacuum radiation field and therefore does not decay spontaneously. Numerical simulations involving different dipole orientations and interatomic distances are present and their subradiance properties are investigated as well.

Spectroscopy of gold atoms in helium nanodroplets

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The $6p \ ^2P_{1/2} \leftarrow 6s \ ^2S_{1/2}$ and $6p \ ^2P_{3/2} \leftarrow 6s \ ^2S_{1/2}$ transitions (D lines) of gold atoms embedded in superfluid helium nanodroplets have been investigated using resonant two-photon ionization spectroscopy. Both transitions are strongly blue-shifted and broadened due to the repulsive interaction between the Au valence electron and the surrounding helium. The assignment of the observed spectral features is supported by ab-initio calculations. The recorded in-droplet D lines are superimposed by the spectral signature of Au atoms relaxed into the metastable 2D states. These features are narrower than the in-droplet D lines and exhibit sharp rising edges that coincide with bare atom transitions. It is concluded that they originate from metastable 2D state $AuHe_n$ exciplexes that have been ejected from the helium droplets during a relaxation process. Interestingly, the mechanism that leads to the formation of these complexes is suppressed for very large helium droplets consisting of about 2×10^6 He atoms, corresponding to a droplet diameter on the order of 50 nm.

Our experiments reveal insight into complex droplet mediated relaxation dynamics, which play an important role in the case of Au atoms and have a strong influence on the observed spectra. An understanding of isolated Au atoms provides a foundation for the study of larger Au clusters in helium droplets towards which our current efforts are geared.

CONDENSED MATTER

(COND)

COND SESSION I 14:00-15:30 TUESDAY, SEP 11

HS P2

COND-1 TALK 14:00-14:15 TUESDAY, SEP 11

HS P2

QWIPs and QCDs for RF

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Optical frequency combs were initially developed in the near infrared region, based on fundamentally mode-locked lasers. Nowadays, large efforts are being made to bring frequency comb technology into the mid-infrared spectral region with a similar degree of maturity. Typical Fabry-Perot QCLs have cavity lengths between 2 and 6 mm resulting in a repetition frequency around 10 GHz. One needs therefore detectors with a bandwidth larger than the repetition frequency to investigate the locking mechanism of the QCLs. In 2006 it was shown that photovoltaic quantum cascade detectors (QCD) show a comparatively flat frequency response up to 4 GHz limited only by the circuit used to contact the detector [1]. With this principle, it was already demonstrated that mid-IR detectors based on intersubband transitions can cover up to 30 GHz of bandwidth [2].

We demonstrate the connection of the QWIP to commercial available RF connectors with a coplanar waveguide. By calculating the gap width of the CPW as function of the center conductor while trying to maintain the characteristic impedance of 50 Ohm, it is possible to suppress reflections due to impedance mismatches. We examined the frequency response of the QWIP by injecting an AM radiofrequency signal into the microwave CPW and sweeping the carrier frequency. The measurement of the rectified signal reveals a cut-off frequency around 10 GHz. Furthermore, we show that it is possible to measure the RF beatnote created by the beating of the Fabry-Pérot modes of a 4 mm long interband cascade laser with an SNR exceeding 15 dB using our RF QWIP at 80 K. We report on a single-period QCD with a room-temperature quantum efficiency of 40 percent and a responsivity of 0.86 A/W [3]. The frequency cut-off around 500 MHz is high enough to cover the highest frequency of the multiheterodyne beatings.

[1] Hofstetter D., Graf M., Aellen T., Faist J., Hvozدارa L., & Blaser S. (2006). 23 GHz operation of a room temperature photovoltaic quantum cascade detector at $5.35\ \mu\text{m}$. *Applied physics letters*, **89**(6), 061119.

[2] Liu H. C., Li J., Buchanan M., & Wasilewski Z. R. (1996). High-frequency quantum-well infrared photodetectors measured by microwave-rectification technique. *IEEE journal of quantum electronics*, **32**(6), 1024-1028

[3] Schwarz, B., Reininger P., Harrer A., MacFarland D., Detz H., Andrews A.M., Schrenk W. and Strasser G. (2017). High-frequency quantum-well infrared photodetectors measured by microwave-rectification technique. *Applied Physics Letter*, **111** (6) 1024-1028

Quantum Cascade Laser and Detector Material Systems

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Quantum cascade lasers (QCL) and detectors (QCD) enable spectroscopy in the MIR and THz finger print regions, spanning 3–300 μm . The material systems used and the band structure engineering they enable determine the properties of intersubband devices. The cubic III-V material systems have been dominant, due to the availability of high quality substrates (GaAs, InP, InAs, GaSb), lattice-matched or strain-compensated barriers, various conduction band offsets (CBO), low electron effective mass m_e^* , and available wave guiding. Large CBOs and a high barrier effective mass m_e^* are helpful for creating short wavelength QCLs and QCDs. However, to improve long wavelength emission, up to the reststrahlen band and above it in the THz range, the large CBO and m_e^* leads to 1-2 monolayer (ML) thick barriers that are challenging to grow uniformly and reproducibly. InAs and InGaAs are the lowest m_e^* well materials, so lattice-match III-AsSb have been developed to tune the CBO and m_e^* .

Symmetric THz QCLs have proven to be an excellent method to study material and interface quality, as well as dopant migration. Interface quality and asymmetry can be compared by the changes in the L-I-V curves for the two bias directions. This allows the identification of higher quality normal InGaAs-to-InAlAs and inverted InAlAs-to-InGaAs interfaces. For InAs/AlAsSb THz QCLs, the AlAsSb barriers are 1-2 ML and lead to more scattering, while 4 ML barriers are suitable for MIR QCDs. In the quest to improve III-AsSb materials, like GaAsSb and AlAsSb, the As-for-Sb exchange becomes a significant factor in growth crystal quality, alloy composition, and lattice matching.

We will present the growth and progress made in materials for MIR and THz devices, including which material system can be used reliably to reach 190 K pulse operations for THz QCLs.

Surface emitting ring interband cascade lasers

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Interband cascade lasers (ICLs) [1,2] combine the concept of quantum cascade lasers (QCLs) and conventional photodiodes, because they rely on the voltage-efficient in-series connection of multiple active regions as in QCLs as well as the long upper-level recombination lifetimes of photodiodes. The distinctive low power consumption of ICLs makes them suitable candidates for compact mid-IR

devices for process control, medical applications and spectroscopy [3].

This work presents special ICL-devices for spectroscopic applications. As a first proof of principle we present ICLs fabricated into ring-shaped cavities [4]. The light is outcoupled in vertical direction through the GaSb substrate using second order distributed feedback (DFB) gratings. The first demonstrated devices with 400 μm outer diameter and a waveguide width of 10 μm show light emission at a wavelength of $\sim 3.7 \mu\text{m}$. A pulsed threshold current density $< 1 \text{ kA/cm}^2$ is measured at 20°C.

We use our devices for trace gas sensing by the principle of $2f$ -wavelength modulation Fabry-Pérot photothermal interferometry and show first results with ICLs in contrast to previous measurements using QCLs [5].

Additionally, we also investigate the suitability of related QCL-concepts to implement them to our ring ICLs (e.g. 2D DFB QCL arrays [6]).

- [1] R. Q. Yang, Infrared laser based on intersubband transitions in quantum wells, *Superlattices Microstruct.* **17**, 77 (1995).
- [2] I. Vurgaftman, R. Weih, M. Kamp, J. R. Meyer, C. L. Canedy, C. S. Kim, M. Kim, W. W. Bewley, C. D. Merritt, J. Abell and S. Höfling, Interband cascade lasers, *J. Phys. D: Appl. Phys.* **48**, 123001 (2015).
- [3] R. Weih, L. Nähle, S. Höfling, J. Koeth, and M. Kamp, Single mode interband cascade lasers based on lateral metal gratings, *Appl. Phys. Lett.* **105**, 071111 (2014).
- [4] M. Holzbauer, R. Szedlak, H. Detz, R. Weih, S. Höfling, W. Schrenk, J. Koeth, and G. Strasser, Substrate-emitting ring interband cascade lasers, *Appl. Phys. Lett.* **111**, 171101 (2017).
- [5] J. P. Waclawek, V. C. Bauer, H. Moser, and B. Lendl, $2f$ -wavelength modulation Fabry-Perot photothermal interferometry, *Opt. Express* **24**, 28958-28967 (2016).
- [6] E. Mujagić, C. Schwarzer, Y. Yao, J. Chen, C. Gmachl, and G. Strasser, Two-dimensional broadband distributed-feedback quantum cascade laser arrays, *Appl. Phys. Lett.* **98**, 141101 (2011).

COND-4 TALK 14:45-15:00 TUESDAY, SEP 11

HS P2

Diagrammatic Monte Carlo study of Fröhlich polaron dispersion in two and three dimensions

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The Diagrammatic Monte Carlo (DMC) is a powerful method which has proven to work in many applications for many different systems. It makes use of diagrammatic expansions of Green's functions and a Metropolis sampling algorithm to perform a random walk in the space of all Feynman diagrams.

For this paper, we have implemented a DMC code based on the approach by Mishchenko et al.¹ and applied it to the solution of the large polaron Fröhlich Hamiltonian in three (3D) and two dimensions (2D). We benchmarked our code with existing DMC results for the 3D case to verify its correctness and then computed polaron ground state energies, effective polaron masses and polaron dispersion curves in 2D and 3D. The results are compared to analytically known limits and to other numerical results from the literature.

Our data confirm that the effect of electron-phonon coupling is enhanced when going from 3D to 2D systems, and this is reflected in all computed physical quantities. The calculated ground state energies from our DMC code are in very good agreement with Feynman's path integral approach

and with exactly known limits in the weak- and strong coupling regime. We further show complete polaron dispersion curves. The DMC calculations reproduce very well the different behavior seen in 2D and 3D: in 2D the energy curve approaches the continuum edge asymptotically from below, whereas in 3D it reaches the continuum edge at a finite critical wave vector. The accuracy of the obtained polaron dispersions is verified with very narrow upper and lower bounds.

[1] A.S. Mishchenko *et al.*, *Phys. Rev. B* **62**, 6317 (2000)

COND-5 TALK 15:00-15:15 TUESDAY, SEP 11

HS P2

Three Dimensional Nanostructuring of Silicon

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Silicon nanostructures have attracted lots of interest for their outstanding and tunable optoelectronic properties. Three dimensional control over their geometry is expected to lead to significant advances in a variety of fields such as photonics, solar fuel generation, photovoltaics or sensing. Unfortunately, this is still a difficult task. We will report on our recent progress to control the growth of well-defined metal nanostructures around single crystalline nanowires produced via metal assisted chemical etching (MACE).¹ The technique is based on simple chemical and electrochemical approaches that were developed previously² and can produce homogeneous large scale (ca. 25mm²) metal-silicon wire arrays with a sub-10 nm resolution.

[1] F. J. Wendisch, R. Oberreiter, M. Salihovic, M. S. Elsaesser, and G. R. Bourret, *ACS Appl. Mater. Interfaces* **2017**, 9, 3931-3939

[2] T. Ozel, G. R. Bourret and C. A. Mirkin *Nat. Nanotech.* **2015**, 10, 319-324

COND-6 TALK 15:15-15:30 TUESDAY, SEP 11

HS P2

Mode-locked interband cascade lasers

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In this work, we demonstrate a frequency comb source based on actively mode-locked interband cascade lasers (ICL), thereby solving two current issues connected to on-chip miniaturization. By utilizing ICLs, we move to a technology with a much smaller power requirement and thermal dissipation to enabling battery driven miniaturized sensors in future. Simultaneously, ICL technology allows straightforward on-chip detection capabilities [1].

Optical frequency combs are light sources whose spectra consist of equally spaced modes. Frequency combs based on QCLs were one of the first compact source in the mid-infrared [2] and their large potential for spectroscopic applications is already evident [3, 4]. We utilize a two-section device consisting of a long gain and a short absorber section that is optimized for RF injection. Active modulation of the short absorber section allows control over the cavity loss and, together with the

long upper state lifetime of ICLs, enables to lock the modes of the cavity to obtain picosecond pulse emission. Observing a narrow beatnote at the round trip frequency can serve as a first indication that at least some of the modes emitted by the laser possess a fixed phase relation.

A much better technique is the so called intermode beat spectroscopy [2]. Thereby, an interferogram of the optical beatnote signal is recorded using a fast detector and a RF spectrum analyzer. It allows to measure the spectrally resolved coherence and thus is a perfect technique to proof frequency comb generation. To proof mode-locking we go one step further and apply a phase sensitive technique to obtain both the amplitude and phase of the beating between each pair of frequency comb lines. Also referred to as shifted wave interference Fourier transform spectrum (SWIFTS) [5], this method allows the reconstruction of the time domain signal emitted by the laser and thus gives a clear proof that our laser is a fundamentally mode-locked frequency comb.

[1] H. Lotfi, L. Li, S. M. S. Rassel, R. Q. Yang, C. J. Corrège, M. B. Johnson, P. R. Larson, and J. A. Gupta, "Monolithically integrated mid-IR interband cascade laser and photodetector operating at room temperature," *Applied Physics Letters* **109**, 151111 (2016).

[2] A. Hugi, G. Villares, S. Blaser, H. C. Liu, and J. Faist, "Mid-infrared frequency comb based on a quantum cascade laser," *Nature* **492**, 229-233 (2012).

[3] G. Villares, A. Hugi, S. Blaser, and J. Faist, "Dual-comb spectroscopy based on quantum-cascade-laser frequency combs," *Nature Communications* **5**, 5192 (2014).

[4] <https://irsweep.com>.

[5] D. Burghoff, Y. Yang, D. J. Hayton, J.-R. Gao, J. L. Reno, and Q. Hu, "Evaluating the coherence and time-domain profile of quantum cascade laser frequency combs," *Optics Express* **23**, 1190 (2015).

COND SESSION II 16:00-17:30 TUESDAY, SEP 11

HS P2

COND-7 TALK 16:00-16:15 TUESDAY, SEP 11

HS P2

In-Situ Studies on the Formation and Tunable Properties of Nanoporous Metals Produced by Electrochemical Dealloying

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Dealloying is a selective (electro-)chemical etching process, which removes the less noble component from an alloy, resulting in a sponge-like structure of the more noble component [1]. In such a way, nanoporous (np) metal structures can be generated in quasi unrestrained (three dimensionally macroscopic) shape, which are attractive for basic research as well as technology applications such as sensing, energy storage or catalysis.

The formation of the nanoporous structure during dealloying is studied by in-situ resistometry, thus providing the first dynamical method for monitoring the etching of macroscopic samples. Using np-Au and np-Pt as examples, we find a resistance increase by about three orders of magnitude due to porosity evolution and concomitant oxide formation. We introduce a model, which allows an evaluation of the etching front propagation ('primary dealloying') as well as the status of the already porous structure ('secondary dealloying'). [2]

Electrochemical property tuning following the concept of Gleiter et al. [3] is particularly promising for dealloyed nanoporous metals due to the high achievable specific surface areas up to $30\text{m}^2/\text{g}$ (np-Pt). By electrochemical ad-/desorption, which strongly influences interfacial charge carrier scattering, reversible variations in the electrical resistance up to several tens of percents can be generated [4]. Moreover electrochemical charging also introduces changes to the atomic bonds in the solid's surface, leading to an actuator behavior of the nanoporous metals. Upon applying potential variations of less than 1 Volt, length changes of more than 0.5% can be achieved reversibly in the case of nanoporous platinum.

[1] J. Erlebacher et al., *Nature* **410** (2001) 450

[2] E. Steyskal et al., *Phys. Chem. Chem. Phys.* **19** (2017) 29880

[3] H. Gleiter et al., *Acta Mater.* **49** (2001) 737

[4] E. Steyskal et al., *Langmuir* **32** (2016) 7757

COND-8 TALK 16:15-16:30 TUESDAY, SEP 11

HS P2

Characterisation of CuZr-based bulk metallic glasses after structural rejuvenation by severe plastic deformation

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Bulk metallic glasses (BMGs) are a fascinating new class of materials with exceptional mechanical properties such as e.g. high hardness combined with high elastic limit. The properties of BMGs are directly linked to their non-crystalline atomic structure lacking long-range order. Since BMGs exhibit also a low ductility caused by a very localized plastic deformation it is one of the challenging aims to fully understand the structure-property relationship in order to find ways and processes for improvements.

In this work we show that severe plastic deformation of BMGs under constrained conditions facilitates a rejuvenation of the disordered atomic structure that impacts the mechanical properties of the processed material. The characterisation of the BMG was accomplished by various methods including Synchrotron X-ray diffraction, nanoindentation, differential scanning calorimetry, atomic force and transmission electron microscopy.

The experimental results clearly show that severe plastic deformation using high-pressure torsion modifies the disordered structure by increasing the mean atomic volume compared to the as cast material. The resulting excess free volume affects also the flexibility of atoms calculated by the mean square atomic displacement and consequently the mechanical properties. The amount of free volume determines the level of rejuvenation that is enhanced at higher shear strains. By a unique and unprecedented mapping of structural and mechanical quantities on micrometer scale a clear correlation both between elastic and plastic softening and between softening and excess free volume can be revealed. In addition, based on the nanoindentation curves it can be concluded that structural rejuvenation promotes a more homogeneous like deformation. Therefore, controlling structural rejuvenation facilitates elastic and plastic properties within a given range.

Quantitative analysis of the precipitation kinetics in dilute alloys by isothermal in-situ high-precision dilatometry

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High-precision dilatometry serves as sensitive tool for quantitatively characterizing precipitation processes even if they are associated with only tiny relative length changes in the range of 10^{-5} and even if they occur on long time scales exceeding 10^5 s. For a dilute Al-based Al-Mg-Si alloy the amount of the metastable coherent β'' -phase and the semicoherent β' -phase as well as of the stable phase β could be determined on an absolute scale from in-situ relative length change measurements upon long-time isothermal annealing.

The quantitative analysis allows an assessment on the various contributions of the length change, i.e., the volume excess of the precipitates, the volume change of the matrix upon precipitation of solute atoms, and the length change due to the formation of interfaces.

The time- and temperature-dependence of the length change could quantitatively be analysed in the framework of the Johnson-Mehl-Avrami-Kolmogorow model, which yields a detailed understanding of the precipitation kinetics. Bringing together all those findings, the industrial highly relevant time-temperature-precipitation diagrams, which, for these types of alloys, were hard to ascertain with common experimental techniques, are now easily accessible.

Electrochemical Tuning of Magnetism in Nanoporous Systems - Oxidation, Hydrogenation and Surface Charging

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Nanoporous materials have attracted considerable interest in the scientific community as functional materials with a broad variety of applications, including catalysis and sensing. Owing to their high surface-to-volume ratios it is possible to alter bulk properties via surface modifications.

Electrochemical reactions represent a versatile method to achieve defined surface states with controlled chemical composition and charging state. Magnetic properties of metals and alloys are highly sensitive to both chemical environment and electronic structure, which motivated our investigations.

Metal and alloy electrodes were prepared via electrochemical dealloying, a selective dissolution process from binary or ternary alloys, respectively. By exposing the precursor to an etching agent, the least noble component of the alloy is gradually removed, while enhancing the surface diffusivity of the more noble compound(s) [1]. Appropriate processing conditions enable the formation of nanoporous structures, with the main benefit being adjustable pore sizes. Nanoporous palladium (npPd) and nanoporous copper-nickel alloys (npCuNi) were used as model systems, amongst other

promising candidates.

Magnetic tuning experiments were performed in an electrochemical cell, designed for special use in a SQUID (Superconducting Quantum Interference Device) magnetometer. This enables sensitive *in situ* measurements of the changes in magnetic moment upon various electrochemical treatments and a direct assignment of chemical reactions to magnetic behaviour [2].

Alterations of the magnetic moment of more than 20% were measured for npCuNi upon surface oxidation in aqueous electrolyte, which will be discussed in terms of a perturbation of the magnetic order of the nickel atoms. Furthermore, changes in magnetisation upon surface charging and hydrogenation of npPd are presented.

This work is financially supported by the Austrian Science Fund (FWF): P30070-N36.

[1] I. McCue et al., *Ann. Rev. Mater. Res.* **46** (2016) 263

[2] E.-M. Steyskal et al., *Beilst. J. Nanotech.* **4** (2013) 394

COND-11 TALK 17:00-17:15 TUESDAY, SEP 11

HS P2

Viscoelastic properties of pulp fibers investigated by atomic force microscopy

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It is well known that paper fibers are an inhomogeneous and hierarchical material. Resulting structure-property relations on the fiber scale as well as on the paper scale are complicated and not yet fully understood. To gain more insight on how mechanical properties of cellulose fibers are related to properties of the paper, our work focusses on the transverse viscoelastic behavior of single pulp fibers investigated. To reach this goal we implemented an atomic force microscopy (AFM) based method. Although AFM is most often used to investigate surface morphology, the AFM probe is also an excellent force sensor. Pulp fibers have not only anisotropic properties, but also a very rough surface which can cause uncertainties in measurements due to not well-established contact between the AFM tip and the fiber surface. For this reason, an AFM method [1] was developed to overcome the surface roughness of the pulp fibers and to determine the viscoelastic properties of single fibers in the transverse direction. The evaluation of the experimental data combines contact mechanics and viscoelastic models. Those models consist of springs and dashpots describing elastic and viscous behavior. Here, it will be demonstrated that the so-called Generalized Maxwell model yields reasonable results for single pulp fibers at different relative humidity values. The values for both, the elastic and viscous parameters decrease with increasing relative humidity.

[1] C. Ganser, et al. *Soft Matter* **14** (2018) 140-150.

Towards a reliable description of lattice vibrations in organic molecular crystals: Effect of van der Waals interactions

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A detailed benchmark of different van der Waals (vdW) methods to describe lattice vibrations of organic molecular crystals in the framework of density functional theory (DFT) will be presented. The performance of the vdW methods was evaluated by comparing calculated and measured lattice Raman spectra in the low-wavenumber region ($< 150 \text{ cm}^{-1}$) of a pool of organic molecular crystals. This region is typically dominated by intermolecular vibrations dependent on vdW interactions, and is therefore suitable to evaluate the reliability of the vdW methods. Amongst the tested vdW methodologies, the more reliable and systematic description of the lattice vibrations of organic molecular crystals is provided by the many-body dispersion (MBD) van der Waals method of Tkatchenko et al.¹ and the pair-wise method (D3-BJ) of Grimme et al.² These methods not only provide the best overall agreement with the experimental spectra, but yield consistent descriptions of the vibrational properties of the studied systems. The accuracy of the other tested approaches (D2³, TS⁴, vdW-DF⁵) is typically lower and varies depending on the system and the wavenumber region. Interestingly, it was found that vdW-free DFT calculations, using structural experimental data, provide lattice vibrations as accurate as those obtained with MBD and D3-BJ.

[1] Tkatchenko, A.; DiStasio, R. A.; Car, R.; Scheffler, M. Accurate and Efficient Method for Many-Body van der Waals Interactions. *Phys. Rev. Lett.* 2012, 108, 236402.

[2] Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* 32, 2011, 1456-1465.

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COND SESSION III 14:00-15:30 WEDNESDAY, SEP 12

HS P2

COND-13 TALK 14:00-14:15 WEDNESDAY, SEP 12

HS P2

Impact ionization processes in the steady state of a driven Mott insulating layer coupled to metallic leads

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We study a simple model of photovoltaic energy harvesting across a Mott insulating gap consisting of a correlated layer connected to two metallic leads held at different chemical potentials [1]. We ad-

dress in particular the issue of impact ionization, whereby a particle photoexcited to the high-energy part of the upper Hubbard band uses its extra energy to produce a second particle-hole excitation. We find a drastic increase of the photocurrent upon entering the frequency regime where impact ionization is possible. At large values of the Mott gap, where impact ionization is energetically not allowed, we observe a suppression of the current and a piling up of charge in the high-energy part of the upper Hubbard band. Our study is based on a Floquet dynamical mean field theory treatment of the steady state with the so-called auxiliary master equation approach as impurity solver. We verify that an additional approximation, taking the self-energy diagonal in the Floquet indices, is appropriate for the parameter range we are considering.

[1] Max E. Sorantin, Antonius Dorda, Karsten Held, and Enrico Arrigoni, *Phys. Rev. B* **97**, 115113 (2018)

COND-14 TALK 14:15-14:30 WEDNESDAY, SEP 12

HS P2

Discrete Transparent Boundary Conditions for the Schrödinger Equation in (1+1)D

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In view of the central importance to quantum physics, accurate and efficient computation schemes for the time-dependent Schrödinger equation are highly desirable. Here we consider a ballistic effective single-electron quantum transport scenario allowing for particle transfer between the simulation region (“device”) and the exterior (“electric contacts”).

We employ unitary higher-order finite difference schemes for the (1+1)D Schrödinger equation. In particular, we address the treatment of open simulation boundaries and develop discrete transparent boundary conditions (TBCs). We first deal with higher-order discretization of the kinetic energy term within the Crank-Nicholson time-propagation scheme. Generalizing earlier work, we find that the dominating growth factor associated with lattice translation in the exterior region suffices to formulate TBCs which suppress reflection from artificial simulation boundaries to basically within machine precision. Furthermore, we argue that, regarding TBCs, increasing the time-accuracy technically is equivalent to increasing space accuracy. Numerical examples are shown.

COND-15 TALK 14:30-14:45 WEDNESDAY, SEP 12

HS P2

Spin- and Valley Polarized Electron Layers

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Charge carriers in semiconductors can have a ‘valley’ degree of freedom, τ . Limited to discrete values (like spin), it can be manipulated by applying mechanical strain. This opens the prospect of valleytronics applications: In addition to the charges, the pseudospin corresponding to a valley’s population is employed for transporting further information. Most promising is to invoke both, τ and the conventional spin σ . We extend the linear response theory for partially spin-polarized electron layers to four-fold degenerate spin-valley systems. There, external electric, magnetic, and mechanical perturbations can independently influence the charge-, spin-, and valley-density,

respectively.

Using the Random Phase Approximation (RPA), we derive all partial and cross-correlation response functions. Their imaginary parts reflect the possible excitations of the system and show a rich structure, depending on momentum transfer $\hbar q$ and energy transfer $\hbar\omega$. In particular, we find a region, where the system is totally non-responsive to applied magnetic fields and mechanical perturbations, similar to the magnetic antiresonance predicted for partially spin polarized systems [1].

[1] D. Kreil, R. Hobbiger, J.T. Drachta, H.M. Böhm, *Physical Review B* **92**, 205426 (2015)

COND-16 TALK 14:45-15:00 WEDNESDAY, SEP 12

HS P2

Collective Modes in Graphene on a Bulk Substrate

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Intensive research on graphene for over a decade has been aimed at improving various existing technologies, spanning the wide range of electrical, optical, thermal, filtering and mechanical applications. In optics, nanophotonic devices require the electromagnetic energy confined to below the diffraction limit, as achieved in plasmonic excitations. Fei et al [1] used scattering-type scanning near-field optical microscopy (s-SNOM) to measure graphene's Dirac plasmon for wave vectors q as large as $3 \cdot 10^9/\text{cm}$. For these collective excitations we here explore the fundamental properties, resulting from the characteristic linear energy dispersion near the high-symmetry-points of the Brillouin zone. First, the complex dielectric function is obtained for freestanding graphene in the random phase approximation (RPA). The large plasmon damping due to interband excitations inevitably leads to the question of how collective modes are properly defined for short lifetimes; we here critically discuss the ambiguous definitions in the literature. Next, the above dielectric function together with that of the substrate is invoked in the calculation of the Fresnel coefficient for p-polarized light reflected by a graphene monolayer on SiO_2 . The interaction with the substrate leads to coupled plasmon-phonon modes, as level-crossings must be avoided.

Finally, we briefly present preliminary studies including spin-orbit coupling (of both, intrinsic and Rashba type). Such contributions to the Hamiltonian split the conduction and valence bands, implying characteristic modifications of graphene's dielectric response function which will, in turn, significantly change the s-SNOM reflectivity.

[1] Z. Fei *et al.*, *Nano Lett.* **11**, 4701 (2011)

Ab initio description of highly correlated states in defects for realizing quantum bitsM. Bockstedte^{1,2}, H. Saßnick¹, F. Schütz², Th. Garratt², Viktor Ivady^{3,4}, A. Gali^{3,5}¹*Department of Chemistry and Physics, University of Salzburg, Salzburg, Austria.*²*Solid State Theory, Friedrich-Alexander University Erlangen-Nürnberg, Germany.*³*Institute for Solid State Physics and Optics, Wigner Research center for Physics, Hungarian Academy of Sciences, Budapest, Hungary.*⁴*Department of Physics, Chemistry, and Biology, Linköping University, Linköping, Sweden.*⁵*Department of Atomic Physics, Budapest University of Technology and Economics, Budapest, Hungary*

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Coupled localized electron spins hosted by defects in semiconductors implement quantum bits with the potential to revolutionize nanoscale sensors and quantum information processing. The present understanding of optical means of spin state manipulation and read-out calls for quantitative theoretical description of the active states, built-up from correlated electrons in a bath of extended electron states. Although the photo physics of a vast variety of systems, including defects, was successfully addressed in the framework of many body perturbation theory (GW and BSE) and time dependent density functional theory, these approaches here do not provide direct access to the important low-spin excited states as well as charge state control via excitations between localized defect states and extended band states.

Here we propose a first-principles scheme based on many body perturbation theory and configuration interaction and address two room temperature point defect qubits, the nitrogen vacancy in diamond, the silicon vacancy, the divacancy, and the nitrogen-vacancy complex in silicon carbide. We provide a complete quantitative description of the electronic structure and analyse the crossings and local minima of the energy surface of triplet and singlet states. Our numerical results not only extend the knowledge of the spin-dependent optical cycle of these defects, but also demonstrate the potential of our method for quantitative theoretical studies of point defect qubits.

Mott physics and transport properties in multi-orbital systems: The example of manganese pnictidesM. Zingl^{1,2}, E. Assmann¹, G. J. Krabberger¹, and M. Aichhorn¹¹*Institute of Theoretical and Computational Physics, Graz University of Technology, Graz, Austria*²*Center for Computational Quantum Physics, Flatiron Institute, New York, USA*

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Strong electronic correlations happen very often in open d- or f-shells close to half filling. As an example of such systems we study BaMn₂As₂ and LaOMnAs, two manganese pnictides. They are similar to the extensively studied iron pnictide high-temperature superconductors BaFe₂As₂ and LaOFeAs, but with the difference of having only 5 electrons in the d shell as compared to 6 electrons in the iron systems. Due to this half-filled situation, the manganese pnictides are candidates for the Mott insulating parent compounds, in analogy with cuprate superconductors. Half-filling has the important consequence that electronic interactions are very effective. As a result, we show that both materials are close to a Mott metal-to-insulator transition, with consequences for their magnetic properties. We calculate optical conductivities as well as Seebeck coefficients for these materials,

and find remarkably good agreement with experimental data. We will relate the large Seebeck effect obtained by the DFT+DMFT calculations to the large asymmetry in the correlated spectral functions.

COND SESSION IV & NESY SESSION I 16:00-17:30 WEDNESDAY, SEP 12 HS P2

NESY-1 TALK 16:00-16:15 WEDNESDAY, SEP 12 HS P2

On Laser Ablation and Injection Moulding as Techniques for the Production of Small Angle X-Ray Scattering Compatible Micro Channels

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We investigated the suitability of different materials and production techniques for producing a micro mixing device to be used in Small Angle X-Ray Scattering (SAXS) experiments. Micro mixers have fast mixing times and low sample consumption and SAXS is a technique well-suited for the characterisation of (macro-) molecular structures. Their combination allows time-resolved investigations of fast reactions, like protein folding. Micro-mixers were already used for SAXS [1], but they were found problematic in some applications, where reaction products can stick to the mixer walls and aggregate, spoiling the data and potentially even clogging the device. 3D-focusing devices [2], which envelope the whole reaction, can prevent the reaction products from reaching the channel walls. This idea is not new, but the intended use in SAXS measurements puts new constraints on the channel where the mixing and measuring occurs. This channel has to be narrow to allow fast mixing and simultaneously deep enough to provide sufficient sample volume for good SAXS measurements.

Moreover, the measurement channel needs to be highly transparent for X-rays for a strong signal and have a low scattering background giving a high signal-to-noise ratio. Both depend on the material and as the scattering signal can be influenced by molecular orientations and stresses induced by the fabrication process, the techniques suitable for producing the mixer are even further limited.

Here we present the results of two methods - laser ablation of polycarbonate [3] and injection moulding of TOPAS [4] - which we found suitable, provided care is taken in aligning the mixing/reaction channel.

This work was supported by the European Commission under grant agreement 654360 NFFA-EUROPE.

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[2] Brennich *et al.*, *Lab Chip* **11** (2011) 708-716

[3] Stratakis *et al.*, *Progress in Quantum Electronics* **3** (2009) 127-163

[4] Petersen *et al.*, *Microelec. Eng.* **133** (2015) 104-109

Revealing the Core/Shell Structure of CdSe/CdS Nanocrystals by synchrotron based SAXS/WAXS studies

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The chemical synthesis of core/shell colloidal nanocrystals (NCs) has led to a pronounced improvement in the optical properties and the chemical stability of semiconducting NCs [1, 2]. The infrared emission of, e.g., lead chalcogenide nanocrystals (NCs) can be drastically increased by stabilising the core with a hard protective shell [1]. For PbS/CdS core/shell NCs we have already shown that metastable crystal phases in a thin, chemical homogenous CdS shell improve significantly the photoluminescence (PL) output of the NCs [3]. This was only achieved by retrieving the chemical profile of NCs in sub-nanometer resolution by using anomalous small angle x-ray scattering (ASAXS) in combination with the analysis of powder diffraction data retrieved by wide angle x-ray scattering (WAXS) [3].

In a current study performed at the synchrotron ESRF, we have investigated CdSe/CdS core/shell NCs with different dimensions by recording simultaneously ASAXS and WAXS spectra. The CdS shells were grown epitaxial on nominal spherical CdSe cores [2]. We revealed that the epitaxial core/shell structure depicts the same sharp chemical interface, even after a post growth annealing step. With increasing NC diameter, however, the CdSe/CdS NCs deviate significantly from a spherical shape. By means of a developed shape retrieval method for SAXS data of colloidal NCs [4], we could reveal an elliptical particle shape with pronounced surface facets for the largest core/shell series. In combination with the recorded powder diffraction data we could relate this anisotropic shape to specific crystallographic directions [5]. The exact understanding of this non-spherical core/shell growth is essential for a precise tuning of the optical properties of CdSe/CdS NCs.

[1] P. Reiss, M. Protiere and L. Liang, *Small* **5**, 154-68 (2009)

[2] O. Chen, J. Zhao, *et al.*, and M. G. Bawendi, *Nature Mater.* **12**, 445-451(2013)

[3] R. T. Lechner, G. Fritz-Popovski, *et al.*, and O. Paris, *Chem. Mater.* **26**, 5914-5922 (2014)

[4] M. Burian, G. Fritz-Popovski, *et al.*, and R.T. Lechner, *J. Appl. Cryst.* **48**,857-868 (2015)

[5] R.T. Lechner, L. Ludescher, D. Dirin, and M. V. Kovalenko, to be published (2018)

Apparent lattice deformation of ordered mesoporous silica during in-situ sorption small angle scattering measurements

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In-situ small angle scattering is a powerful tool to determine adsorption induced deformation in

mesoporous materials exhibiting ordered porosity such as in SBA-15 silica. It has been shown previously, that the change in contrast due to the irregular filling of the mesopores at the pressure of capillary condensation in SBA-15 leads to apparent lattice deformations¹. Recent experiments in our group indicate, that this effect is not restricted to capillary condensation only, but extends to relative pressures below (film regime) and above (filled regime) the pressure of capillary condensation, and severely influences the total strain measured². To study this effect in detail we recorded both, small angle x-ray (SAXS) and neutron (SANS) scattering data of hierarchical, ordered mesoporous silica with different thermal histories. The neutron scattering length density (sld) of the adsorbate water was varied via deuteration, resulting in significantly different strain isotherms for X-rays and neutrons. In particular, for zero-sld, no apparent strains are expected, thus providing the unperturbed strain isotherm.

To simulate the apparent strains, a structural model of the pore space is set up and the adsorption process in the pores is modelled using known theoretical concepts. This is the basis for the form factor put into the Debye equation³ to simulate the scattering data. The apparent peak shift from the ordered pore lattice due to the different loading and scattering contrast is then compared to the experimental data.

[1] Prass, Johannes, et al. "Apparent lattice expansion in ordered nanoporous silica during capillary condensation of fluids." *Journal of Applied Crystallography* **45.4** (2012): 798-806.

[2] Morak, Roland, et al. "Quantifying adsorption-induced deformation of nanoporous materials on different length scales." *Journal of Applied Crystallography* **50.5** (2017).

[3] Debye, Peter. "Zerstreuung von Röntgenstrahlen." *Annalen der Physik* **351.6** (1915): 809-823.

COND-19 TALK 16:45-17:00 WEDNESDAY, SEP 12

HS P2

Magnetoresistance of phase separated (Ga,Fe)N containing $Ga_yFe_{4-y}N$ embedded nanocrystals

A. Navarro-Quezada¹, M. Aiglinger¹, K. Gas², B. Faina¹, M. Matzer¹, Tian Li², R. Jakiela², P. Dluzewski², T. Dietl², M. Sawicki² and A. Bonanni¹

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Gallium nitride (GaN) and related compounds are key material systems in today's optoelectronic and high-frequency technology. When doped with Fe, (Ga,Fe)N undergoes crystallographic phase separation at concentrations above 0.4% of Fe cations, leading to the assembly of Fe-rich embedded nanocrystals (NCs) [1,2]. By fine tuning the growth parameters during a metal-organic vapour phase epitaxy process, the growth of ordered magnetic planar arrays of $Ga_yFe_{4-y}N$ ($0 < y < 1$) NCs embedded in GaN is obtained [3,4].

Here, we analyze the magnetotransport properties of a planar ordering of $Ga_yFe_{4-y}N$ NCs embedded in GaN over the temperature range 2-300 K. The layers show a positive magnetoresistance (MR) above 50 K, while at lower temperatures a mixed behavior of positive and negative MR is observed. The low temperature MR is explained in the frame of the variable range hopping conduction mechanism, with a minor contribution from the embedded ferromagnetic NCs at magnetic fields < 1 T [5]. Furthermore, we find a sizeable anisotropic magnetoresistance as high as 16% at 2 K and 2% at 300 K, which is attributed to the magnetic anisotropy of the planar arrays of $Ga_yFe_{4-y}N$ NCs [4].

The control over spinodal nanodecomposition by growth parameters and the above magnetotransport properties open wide perspectives for the manipulation of the Fe-rich NC's magnetic mo-

ment via an external electric field [6].

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- [2] A. Navarro-Quezada et al., *Phys. Rev. B* **81**, 205206 (2010)
- [3] A. Navarro-Quezada et al. , *Appl. Phys. Lett.* **101**, 081911 (2012)
- [4] A. Grois et al. *Nanotechnology* **25**, 395704 (2014)
- [5] A. Navarro-Quezada et al. unpublished data
- [6] D. Sztenkiel et al. *Nat. Commun.* **7**, 015034 (2017)

COND-20 TALK 17:00-17:15 WEDNESDAY, SEP 12

HS P2

Characterization of Tannin-Furanic Foams by Raman Spectroscopy, Infrared Spectroscopy, and by X-ray Computed Microtomography

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The main goal of this research activity is the characterization of totally natural rigid foams, derived from byproducts of wood industries (such as tannin and lignin) at the nano, micro and macro level through the exploitation of state-of-the-art spectroscopic techniques combined with imaging and mapping options, employing a wide range of electromagnetic radiation from far infrared to X-rays.

The tannin-based foam formation is an acid-catalysed polymerization involving a self-blowing reaction in which the foam raises up introducing a preferential direction of growing. This foam synthesis is a crucial point influencing internal chemical and morphological variations which might affect the macroscopic properties of the foam as final product, since the correlation between structure and degree of pore connection, as well as the chemical nature of the skeleton and surfaces of the walls, play a fundamental role for steering the most appropriate applications. The synergistic complementation of several analytic techniques (Raman spectroscopy, infrared spectroscopy, X-ray microcomputed tomography), available as a cross-border infrastructure via a cooperation between Elettra Sincrotrone Trieste, University of Salzburg and Salzburg University of Applied Sciences within the Interreg Italy-Austria ITAT1023 InCIMA project (2017-2019), will enable to optimize, in future subsequent steps, these materials with potential applications as new materials for green-building technology (e.g. thermal and acoustic isolation) and for natural filtering systems (e.g. water purification from contaminants of emerging concern).

We acknowledge financial support provided by Central European Research Infrastructure Consortium through the proposals CERIC 20167027 and 20177080.

We acknowledge financial support provided by the European Regional Development Fund and Interreg V-A Italy-Austria 2014-2020 through the Interreg Italy-Austria project ITAT 1023 InCIMA <http://www.elettra.eu/Prj/InCIMA/>.

X-ray study of the Hydration of Lipid Membranes upon Interaction with a Mesoporous Support prepared by Deep X-Ray Lithography Technique

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In this communication we present the structural study of the hydration of model lipid membranes fed with water through the porosity of mesoporous substrates prepared by X-ray irradiation using Deep X-ray Lithography (DXRL) technique. The study was conducted using Grazing Incidence Small Angle X-ray Scattering (GISAXS). We wanted to demonstrate the possibility to use mesoporous substrates as “active” sample holders, where porosity is employed to convey liquids. This would enable the use of such films for more complex biological studies by selectively functionalizing the mesopores.

Films were prepared following different recipes and exposed to different X-ray doses at the DXRL beamline at Elettra-Sincrotrone Trieste, resulting in different pore size and arrangement. Time resolved GISAXS measurements were taken on the lipid membrane deposited on the mesoporous films in controlled environment, using a custom made humidity chamber mounted at the Austrian SAXS beamline at Elettra-Sincrotrone Trieste. The first results evidenced partial hydration of the lipid membrane through the mesopores, demonstrating the possibility to use the porosity of the film to convey liquids. Moreover, hydration can be tuned through both the recipe and the irradiation dose of the mesoporous film.

This work was supported the European Commission under grant agreement 654360 NFFA-EUROPE. CERIC-ERIC consortium is acknowledged for the access to experimental facilities.

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[3] B. Marmiroli, H. Amenitsch, *Eur. Biophys. J.* **41**(2012) 851.

EXTREME LIGHT INFRASTRUCTURE

(ELI)

ELI SESSION I	14:00-15:30	WEDNESDAY, SEP 12	SR IF
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ELI-1 TALK	14:00-14:30	WEDNESDAY, SEP 12	SR IF
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ELI: Scientific opportunities, perspectives and challenges

D. Charalambidis (on behalf of ELI-DC)

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Large international research infrastructures have over many decades promoted excellence in science and technology globally. In the spirit of this international practice, the European Strategy Forum for Research Infrastructures (ESFRI) has developed and keeps updating a roadmap for European Research Infrastructures (RIs). The Extreme Light Infrastructure (ELI) has been included in the ESFRI Roadmap published in 2006. During the EU funded project “ELI preparatory phase” (2007-2011) it was decided that ELI will be implemented as a distributed infrastructure in: Szeged, Hungary [ELI-Attosecond Light Pulse Source (ELI-ALPS)], Dolní Břežany, Czech Republic [ELI-Beamlines (ELI-BL)] and Magurele, Romania [ELI-Nuclear Physics (ELI-NP)]. ELI enters its operation phase in the three Host Countries starting in 2018 as a Pan-European RI with a common governance and access policy through the under establishment ELI- European Research Infrastructure Consortium (ELI-ERIC).

The three geographically separated ELI Facilities, each serving a distinct mission, will form the most unique and advanced user-based laser facility of its kind in the world, bringing Europe to the lead in this innovative field. ELI supports experiments and the development of the technologies based on extreme light-matter interactions at the highest intensities, shortest time scales and broadest spectral range. The RI aims for multidisciplinary scientific and technical applications, including:

- Basic and applied research goals in physical, chemical, material and life sciences
- Visualization of ultrafast structural dynamics
- Strong-field quantum electrodynamics and associated vacuum effects
- A combination of laser and accelerator technologies to investigate plasma physics, nuclear structure and reactions, as well as nuclear astrophysics with unprecedented precision and accuracy
- Bringing together important scientific communities - laser, nuclear and astrophysics - to realize an integration of the disciplines to stimulate development of the new field of nuclear photonics.

This presentation highlights the main technologies to be provided by ELI as well as the scientific opportunities and future perspectives ELI opens to the international scientific community.

Few-cycle laser based research technologies for users at ELI Attosecond Light Pulse Source

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Five major laser systems are being implemented at the Attosecond Light Pulse Source (ALPS) facility of the pan-European Extreme Light Infrastructure (ELI), operating in different regimes of repetition rate, peak power, and spectral range. All sources deliver pulses with unique parameters: unparalleled fluxes, extreme broad bandwidths and sub-cycle control of the generated fields.

The HR1 and HR2 lasers combine fiber laser technology with HCF pulse compression, offering 0.2-1 TW peak power, sub-6fs pulses around 1030 nm with 100 kHz repetition rate. They are synchronized at the same rate with the mid-infrared laser (MIR), providing four-cycle pulses at 3 micron with an average power of 15 W. The SYLOS system relying on OPCPA generates 2 cycle laser pulses at 1 kHz repetition rate, with a stability of <1% rms. The hybrid high-field (HF) laser will operate at 10 Hz repetition rate with 17 fs pulse duration, reaching a peak power of 2 PW.

The performance of the laser sources will enable the generation of secondary sources with exceptional characteristics, including light sources ranging from the THz to the X-ray spectral ranges and particle beams. Among them, the primary focus of ELI-ALPS is the generation of the best quality XUV attosecond pulses in terms of pulse energy, repetition rate and photon energy. High flux attosecond pulse trains and isolated attosecond pulses are targeted via high harmonics in gases and plasmas. The secondary source beamlines will be equipped with a set of diagnostics enabling the users to perform experiments as COLTRIM, APRES, VMI, etc.

The first commissioning experiments have been kicked off with the commissioning of the MIR and the HR laser systems in January 2018. Simultaneously, we have also started the assembly of the high harmonic beamlines, the THz laboratory, and nanoplasmonic experiments. The first XUV bursts of light with attosecond duration are expected to be generated by the end of 2018. The operation of each source and target area station is planned to start gradually, the last one reaching the (external) user readiness status by mid 2021.

Attosecond measurement and control of electron and nuclear dynamics in molecules

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When an intense laser pulse impinges on a molecule, the laser electric field couples to the molecular electronic system and can drive various ultrafast electronic processes that may reach into the attosecond time domain. The laser-field-induced distortions of the molecular electronic system might leave the molecule in an (ionic) electronically and/or vibrationally excited state (and superpositions of them), which in turn may give rise to nuclear dynamics that typically takes place on considerably longer time-scales ranging from about ten femtoseconds to picoseconds. While a number of methods for the measurement of attosecond electronic dynamics have been developed, e.g., intra-cycle interferometry with electron wavepackets [1], it is difficult to capture simultaneously both the fast electronic and the slower nuclear motion.

In this talk I will introduce, using the H₂ molecule as an example, a method that closes this gap.

This method, termed attosecond molecular clock, exploits the concept of angular streaking for which the absolute values of the momenta of the electrons and their emission angles, associated with the hour respectively the minute hand of the clock, encode the release times of the electrons [2]. To obtain absolute timing, the clock needs to be calibrated by the carrier-envelope phase (CEP) of the laser pulses [2]. To apply the clock to molecules, an additional hand for encoding the nuclear motion that may take place during double ionization needs to be added. We show that the kinetic energy release (KER) can serve as this hand of the clock. Using the resulting molecular attoclock we experimentally trace the sub-cycle dynamics of two-electron emission from H₂ that underlies the fragmentation dynamics into two protons.

I will furthermore show that this molecular attoclock can also provide new insight into the charge-localization process that takes place during dissociation of H₂⁺ into a proton and a neutral hydrogen. Our measurements reveal that in an elliptically polarized laser field with field components in two spatial dimensions, the charge-localization is determined and can ultimately be controlled by a combination of three parameters: the CEP of the laser field, the ionization phase, and the molecular alignment. While the CEP influences the charge-localization in the lab-frame, the ionization phase is effective in the molecular frame of reference. The molecular alignment is the parameter that connects both frames of reference. Thus, a given combination of these three parameters completely determines the charge-localization process.

[1] X. Xie *et al.*, *Phys. Rev. Lett.* **108**, 193004 (2012)

[2] M. Schöffler *et al.*, *Phys. Rev. A* **93**, 63421 (2016)

ELI-4 TALK 15:10-15:30 WEDNESDAY, SEP 12

SR IF

Probing Nanoplasmonic Field Enhancement with Ultrafast Photoemission

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Probing optical near-fields quantitatively is a major challenge in nanoscale photonics and plasmonics. We show that measuring the electron energy in ultrafast photoemission allows to deduce the maximum field enhancement in any metallic surface environment [1]. In general, photoemission induced by femtosecond laser pulses opens a view into the processes of electron emission and acceleration in highly confined optical fields [2].

[1] P. Racz, Z. Papa, I. Marton, J. Budai, P. Wrobel, T. Stefaniuk, C. Prietl, J.R. Krenn, P. Dombi, *Nano Lett.* **17**, 1181 (2017)

[2] P. Dombi, A. Hörl, P. Racz, I. Marton, A. Trügler, J.R. Krenn, U. Hohenester, *Nano Lett.* **13**, 674 (2013)

ELI-5 TALK 16:00-16:30 WEDNESDAY, SEP 12

SR IF

Extreme Light Infrastructure (ELI): Science and Technology at the ultra-intense Frontier

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We will be giving an overview on the development of the “ELI-beamline facility” being built within the Extreme Light Infrastructure (ELI) project based on the European ESFRI (European Strategy Forum on Research Infrastructures) process.

ELI-Beamlines will be a high-energy, repetition-rate laser pillar of the ELI (Extreme Light Infrastructure) project. It will be an international facility for both academic and applied research, slated to provide first user capability in 2018. The main objective of the ELI-Beamlines Project is delivery of ultra-short high-energy pulses for the generation and applications of high-brightness X-ray sources and accelerated particles. The laser system will be delivering pulses with length ranging between 10 and 150 fs and will provide high-energy Petawatt and 10-PW peak powers. For high-field physics experiments it will be able to provide focused intensities attaining 10^{24} Wcm⁻², while this value can be increased in a later phase without the need to upgrade the building infrastructure to go to the ultra-relativistic interaction regime in which protons are accelerated to energies comparable to their rest mass energy on the length of one wavelength of the driving laser. The major directions of the high field Physics program and the first anticipated experiments will be described.

Furthermore, we will discuss the development of the laser program and secondary sources of particles and x-rays in the wavelength range between 20 eV - 100 keV - few MeV and their practical implementation as beamlines in the ELI-beamline user facility. The sources are either based on direct interaction of the laser beam with a gaseous or solid target or will first accelerate electrons which then will interact with laser produced wigglers (Betatron radiation) or directly injected into undulators (laser driven LUX or later X-FEL). The direct interaction (collision) of laser accelerated electrons with the laser again will lead to short pulse high energy radiation via Compton or Thomson scattering allowing to perform fundamental Physics investigation of laser particle interaction.

ELI-6 TALK 16:30-16:50 WEDNESDAY, SEP 12

SR IF

Where does ELI-NP stand now?

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Since chirped pulse amplification scheme [1] deployed in high intensity laser systems has altered the games in high energy density physics, the focusable laser intensity has kept increasing and can reach 10^{23} W/cm². Using these laser systems one can obtain relativistically accelerated electrons and protons as well as intense gamma beams whose energy is higher than the previously used in nuclear facilities. In order to make use of this capability in full depth, ELI-NP has been funded to come up

with both high intensity laser and high brilliance gamma beam systems through the European Light Infrastructure (ELI) project for the state of the art and beyond and approaches to its full operation.

The high power laser system (HPLS) consists of OPCPA, Ti Sapphire configuration at the central wavelength 820 nm with 60 nm bandwidth, the output energy 250 J, the pulse width 25 fsec, the contrast ratio 10^{13} with 50 cm beam diameter. This may enable to create a focused laser intensity $10^{22} - 10^{23}$ W/cm² on target. 3 PW performance test has been successfully achieved in May 2018.

The output of gamma beam system (GBS) comes up with continuously tunable energy in the range from 200 keV to 19.5 MeV with 109 photons/sec after the slit. The production of quasi-monochromatic gamma beams is based on the Inverse Compton Scattering (ICS) process of green laser light pulses off relativistic electron bunches up to 700 MeV. The resulting GBS is based on a high-quality electron-photon collider with luminosity at the level of about 2×10^{35} cm⁻²s⁻¹, that is almost one order of magnitude better than what was achieved at LHC in CERN [2].

The commissioning phase may be expected to start as early as in 2018. A number of experiments have been proposed for the Day 1 phase and has been recommended by the International Scientific Advisory Board (ISAB). For example gamma ray conversion efficiency, high energy electron acceleration, and non-linear QED [3] are being prepared for the HPLS. First-phase experiments for the GBS involve studies of the distribution of the E1 strength in the region of the Pigmy Dipole Resonance (PDR) and the Giant Dipole Resonance (GDR). Delbrück Scattering is also considered. These experiments will take advantage of the narrow-bandwidth pencil-size beams at ELI-NP, which provide the possibility for studies low-abundance targets, e.g. NRF studies in the actinide nuclei. Most recent status with details will appear soon [4].

[1] D. Strickland and G. Mourou, "Compression of amplified chirped optical pulses", *Opt. Commun.* **56**, 219 (1985).

[2] D. Balabanski, R. Popescu, D. Stutman, K. A. Tanaka, O. Tesileanu, C. A. Ur, D. Ursescu and N. V. Zamfir, "New light in nuclear physics: The extreme light infrastructure", *European Phys. Lett.* **117**, 28001 (2017).

[3] N. V. Zamfir *et al.*, *Romanian Reports in Physics*, Vol. **68**, Supplement I & II, 2016.

[4] S. Gales *et al.*, "Extreme Light Infrastructure - Nuclear Physics pillar (ELI-NP) : new horizons in physics with high power lasers and brilliant gamma beams", to appear in *Report on Progress in Physics* 2018.

ELI-7 TALK 16:50-17:10 WEDNESDAY, SEP 12

SR IF

Simulation of EUV mirrors towards all-angle reflection

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Future lithography will require optics for radiation in the extreme ultraviolet, e.g. produced by a Sn plasma at 13.5 nm. At this wavelength mirrors using multilayer structures are required. The basic structure consists of alternating layers of Mo and Si. In this work modifications to this structure to change the width of the reflectivity spectrum, and the region of incident angles, where strong reflection occurs, are studied.

This investigation is performed by simulations of the reflectivity using the transfer matrix method which describes the interaction of each layer with the incident and out-going waves by a scattering transfer matrix. The properties of the total system are given by the product of the individual matrices. For arbitrary three-dimensional structures the finite difference time domain (FDTD) method which discretizes the Maxwell equations can be used.

Using superlattices, where every n -th (e.g. every 5th) Mo layer is replaced by Si, and by splitting the multilayer structures into regions with different layer widths the range of angles reflecting can be widened. It is even possible to achieve (for polarization parallel to the layer planes) all-angle reflection. As a trade-off, the peak reflectivity is reduced.

NUCLEAR and PARTICLE PHYSICS

(FAKT)

FAKT SESSION I 14:00-15:30 WEDNESDAY, SEP 12

SR TDK

FAKT-1 TALK 14:00-14:25 WEDNESDAY, SEP 12

SR TDK

Imaging with ion beams at MedAustron

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MedAustron is a center for proton and carbon ion beam therapy, and clinical and non-clinical research in Wiener Neustadt. The energy loss of a charged particle is characterized by a sharp peak just before the particle comes to a complete stop. Based on this property, an accurate form of treating deep seated solid cancer using ion beams has been established. However, this requires precise knowledge of the stopping power of the object traversed by the ions. Currently the calculation of this stopping power is mainly based on photon computed tomography, which entails conversion errors. These errors can be reduced by directly measuring the stopping power with the respective ion. Therefore, an experimental program has been started to develop ion beam imaging for a direct measurement of stopping power distributions of charged particles while passing through a phantom.

The prototype currently uses two pairs of position sensitive detector modules which are fixed in a frame. A rotating table that can hold a phantom is placed between the detector pairs, so that ion tracks before and after the phantom can be recorded. Additionally, a calorimeter consisting of a stack of plastic scintillators to stop the ions and measure their residual energies is planned to be put in operation. To trigger the whole system, another pair of scintillators in coincidence, is used.

The raw data produced by the setup are pre-processed and converted to the linear collider I/O (lcio) data format from which detector alignment and particle tracks are obtained by using the EU-Telescope framework. First results produced with our setup in the MedAustron proton beam will be presented and the next steps in the analysis, including a simple reconstruction of the stopping power distribution in the sample, will be discussed.

FAKT-2 TALK 14:25-14:50 WEDNESDAY, SEP 12

SR TDK

Direct Search for Dark Matter with the CRESST-III Experiment

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The ongoing investigation into the nature of dark matter is one of the most prominent fields of

modern physics. A straightforward method is the direct detection approach, where one looks for interactions of hypothetical dark matter particles with a target of ordinary matter such as elastic scattering. In the dark matter particle mass range below $1.7\text{GeV}/c^2$, CRESST-III (Cryogenic Rare Event Search with Superconducting Thermometers) is presently one of the leading experiments worldwide to set exclusion limits on the dark matter particle - nucleus elastic scattering cross section. Located at Laboratori Nazionali del Gran Sasso (LNGS) in Italy, CRESST-III detectors are shielded by a rock overburden of 1400 m and operate in a low background environment. CaWO_4 crystals are used as detector medium and operated as cryogenic detectors at temperatures around 10 mK. In the current operating phase, detector thresholds for recoil energies below 100 eV were achieved, allowing for the exploration of new parameter space. The most recent results from CRESST-III will be presented, as well as an outlook on future development and possible extensions of the experiment.

FAKT-3 TALK 14:50-15:15 WEDNESDAY, SEP 12

SR TDK

Recent Measurements of P-wave quarkonia at CMS

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Although quantum chromodynamics is well established as a theory of strong interactions, the understanding of the nonperturbative processes that bind quarks and gluons into hadrons is still incomplete. Measuring the properties of P-wave quarkonia is an important ingredient to further the understanding of hadron formation. This presentation gives an overview of recent measurements of P-wave quarkonium states using proton-proton collision data taken at the CMS detector at the LHC. The results include the first observation of the $\chi_{b3}(1P)$ and the $\chi_{b3}(2P)$ states and their individual masses.

FAKT-4 TALK 15:15-15:30 WEDNESDAY, SEP 12

SR TDK

Weak Values and Weak Measurements studied in Neutron Interferometry

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Weak measurements [1], introduced exactly 30 years ago, underwent a metamorphosis from a theoretical curiosity to a powerful resource for exploring foundations of quantum mechanics, as well as a practical laboratory tool. However, unlike in the original textbook experiment, where an experiment with massive particles is proposed, experimental applications are realized applying photonic systems. We have overcome this gap by developing a new method to weakly measure a massive particle's spin component. Our neutron optical approach is realized by utilizing neutron interferometry, where the neutron's spin is coupled weakly to its spatial degree of freedom [1]. This scheme was then applied to study a new counter-intuitive phenomenon, the so-called quantum Cheshire Cat: If a quantum system is subject to a certain pre- and post-selection, it can behave as if a particle and its property are spatially separated, which is demonstrated in an experimental test [2,3]. State tomography, the usual approach to reconstruct a quantum state, involves a lot of computational post-processing. So in 2011 a novel more direct method was established using weak measurements. Because of this weakness the information gain is very low for each experimental

run, so the measurements have to be repeated many times. Our procedure is based on the method established in 2011, without the need of computational post processing, but at the same time uses strong measurements, which makes it possible to determine the quantum state with higher precision and accuracy. We performed a neutron interferometric [4] experiment, but our results are not limited to neutrons, but are in fact completely general. In our latest experiment [5] we investigated the paths taken by neutrons in a three-beam interferometer by means of which-way measurements, realized by a partial energy shift of the neutrons so that faint traces are left along the beam path. Final results give experimental evidence that the (partial) wave functions of the neutrons in each beam path are superimposed and present in multiple locations in the interferometer.

[1] S. Sponar, T. Denkmayr, H. Geppert, H. Lemmel, A. Matzkin, J. Tollaksen, and Y. Hasegawa, *Phys. Rev. A* **92**, 062121 (2015).

[2] T. Denkmayr, H. Geppert, S. Sponar, H. Lemmel, A. Matzkin, J. Tollaksen, and Y. Hasegawa, *Nat. Commun.* **5**, 4492 (2014).

[3] S. Sponar, T. Denkmayr, H. Geppert, and Y. Hasegawa, *Atoms* **4**, 11 (2016).

[4] T. Denkmayr, H. Geppert, H. Lemmel, M. Waegell, J. Dressel, Y. Hasegawa, and S. Sponar, *Phys. Rev. Lett.* **118**, 010402 (2017).

[5] H. Geppert, T. Denkmayr, S. Sponar, H. Lemmel, T. Jenke, and Y. Hasegawa, *Phys. Rev. A* **97**, 052111 (2018).

FAKT SESSION II 16:00-17:30 WEDNESDAY, SEP 12 SR TDK

FAKT-5 TALK 16:00-16:15 WEDNESDAY, SEP 12 SR TDK

SModelS: An LHC New Physics Tool - Update to signatures beyond missing energy

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SModelS is a tool designed to decompose Beyond Standard Model (BSM) theories with a Z_2 symmetry and confront them to results from the LHC experiment. The code uses simplified models results to achieve the task in a model independent way. The existing version focuses on supersymmetry searches with missing energy (MET) final state and already includes a large variety of searches from ATLAS and CMS. Ongoing development is aimed at exploring beyond MET signatures of current interest within the theory and experimental community.

I will describe the latest SModelS update which includes upgrading SModelS to a completely object oriented version and thus allows to probe BSM models containing non-MET signatures. The modification facilitates integrating the particles' properties such as mass and life time which is imperative to investigate other signatures. Furthermore, I will present the improved database of experimental results which is extended by adding the latest results from the LHC including searches for Heavy Stable Charged Particles (HSCP). On the basis of these developments I will exemplify the impact of this new SModelS version on new physics scenarios.

Track reconstruction in the CMS experiment for the High Luminosity LHC

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Tracking is one of the crucial parts in the event reconstruction of the Compact Muon Solenoid (CMS) experiment because of its importance in the estimation of particle momenta and decay vertices. This task is challenging at the Large Hadron Collider (LHC), given the hundreds or even thousands of particles generated in each bunch crossing.

In the period from 2024 to 2026, the LHC will be upgraded to the High Luminosity LHC that will provide an unprecedented instantaneous luminosity of $5 - 7.5 \times 10^{34} \text{ cm}^{-2} \text{ s}^{-1}$. This talk will describe the latest developments of the CMS track reconstruction at the HL-LHC using the new silicon-based tracker. Track reconstruction in CMS is developed following an iterative philosophy using an adaptation of the combinatorial Kalman Filter. As a first step, the existing tracking algorithms are adapted to the new detector and the performance for high pileup scenarios are evaluated. This work is reported in “The Phase-2 Upgrade of the CMS Tracker” Technical Design Report. As a successive step, a new type of hits, so-called vector hits, in the outer part of the new tracker are implemented to understand whether they can bring tangible benefits. Their use in tracking and the inclusion of a new iteration, in which seeds are built using only the vector hits, show a reduction of about an order of magnitude of the number of mis-identified tracks and a significant improvement in the reconstruction of tracks coming from displaced vertices.

The CMS High Granularity Calorimeter for the High Luminosity LHCManfred Valentan, on behalf of the CMS collaboration*Institute of High Energy Physics, Austrian Academy of Sciences*

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The CMS experiment at CERN will undergo significant improvements during the so-called Phase-II Upgrade to cope with a 10-fold increase in integrated luminosity with the High Luminosity LHC (HL-LHC) era. The forward calorimetry will suffer from very high radiation levels and intensified pileup in the detectors. The CMS collaboration is designing a High Granularity Calorimeter (HGCal) to replace the existing endcap calorimeters. It features unprecedented transverse and longitudinal segmentation for both electromagnetic (CE-E) and hadronic (CE-H) compartments. This will facilitate particle-flow calorimetry, where the fine structure of showers can be measured and used to enhance pileup rejection and particle identification, whilst still achieving good energy resolution. The CE-E and a large fraction of CE-H will be based on hexagonal silicon sensors produced from 8-inch wafers, each with 192 or 432 individual cells of $0.5 - 1 \text{ cm}^2$ cell size. The remainder of the CE-H will be based on highly-segmented scintillator tiles with on-tile SiPM readout. An overview of the HGCal project is presented in this talk with a focus on the silicon sensors. We cover motivation, engineering design, expected performance and the current status of prototypes: from lab measurements to beam tests.

The CMS Outer Tracker system for the High Luminosity LHC

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The Large Hadron Collider (LHC) is the world's largest particle collider with a center of mass energy of up to 14 TeV. The Compact Muon Solenoid (CMS) is one of its four large experiments. This detector system was designed to search for the Higgs boson and phenomena beyond the standard model of particle physics. The innermost component of CMS is the so-called “Tracker”. Approximately 24000 silicon detectors are used to reconstruct particle trajectories emerging from the interaction point, to measure their momenta in a magnetic field of 3.8 Tesla. During normal LHC operation the Tracker is permeated by the particle flux from the interaction point, leading to irradiation damage on the detector components. The performance of the detector slowly degenerates, eventually compromising the tracking performance beyond acceptable limits. This limit is expected to be reached in the middle of the next decade. Therefore, it will have to undergo an upgrade procedure, which is referred to as the “Tracker Phase-2 Upgrade”.

This upgrade is scheduled between 2024 and 2026 in a period called long shutdown three (LS3). During this phase, the LHC accelerator will be upgraded to the High Luminosity (HL-)LHC, which will lead to a significant increased luminosity. Tracking at high luminosity is substantially more challenging, not only because of the increased particle flux, but also because the performance of selection algorithms degrades with increasing pile-up. Therefore, the capabilities of the new Tracker will be extended with on-chip momenta discrimination. This technique locally rejects events with irrelevant low-momentum tracks and therefore reduces the bandwidth for selection algorithms.

This talk will be comprised of the physics motivation regarding the current and the upgraded Tracker system as well as their limits. Moreover, it will give an in-depth insight into the technological challenges of developing a tracking system for high luminosities in a harsh radiation environment, like at the HL-LHC.

A New High-precision Silicon Drift Detector System for Kaonic Atom Measurements at J-PARC and DAFNE

C. Tripl (on behalf of the E57 and Siddharta-2 collaborations)

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The study of exotic atoms carrying strangeness, e.g. kaons, can provide an answer to the still unsolved question of the generation of hadron masses in a bound system. The proposed kaonic deuterium measurements at J-PARC (see [2], [3]) and DAFNE [4] will provide - in addition to the already performed kaonic hydrogen measurement “SIDDHARTA” at DAFNE [1] - important information for the determination of the isospin dependent scattering lengths a_0 and a_1 . Furthermore, the kaonic helium experiment at J-PARC [5] will give an insight into the possible isotope shift of ^3He and ^4He .

For the kaonic deuterium measurement the shift and width of the $2p \rightarrow 1s$ transition will be determined (with a precision of 60 eV and 140 eV, respectively) by measuring the energy of the transition photon, which will be detected by 48 newly developed Silicon Drift Detectors (SDDs). The SDDs surround a cryogenic target cell filled with gaseous deuterium, providing a total active area of 246 cm^2 .

Several SDD test measurements have been performed at the Stefan Meyer Institute, including

stability tests to guarantee the summing of all 384 channels as well as drift time measurements and crosstalk evaluations. In June 2018, the SDDs will be used at the E62 experiment at J-PARC to determine the X-ray yield of the $3 \rightarrow 2$ transition for kaonic helium, and to study the performance of the SDDs in real beam environment.

- [1] SIDDHARTA Collaboration, *Phys. Lett. B* **704** (2011) 113
- [2] J. Zmeskal *et al.*, *JPS Conf. Proc.* **17** (2017) 071001
- [3] J-PARC proposal E57 (2015)
- [4] H. Shi *et al.*, *Journal of Physics: Conf. Series* **800** (2017) 012007
- [5] T. Hashimoto *et al.*, *JPS Conf. Proc.* **17** (2017) 072001

FAKT-10 TALK 17:15-17:30 WEDNESDAY, SEP 12

SR TDK

A charged particle veto detector for kaonic deuterium measurements at DAΦNE

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The determination of scattering lengths of low-energy antikaon-nucleon interactions provides crucial insight in the non-perturbative regime of QCD, elucidating the process of spontaneous chiral symmetry breaking in hadron physics. Following the kaonic hydrogen results of SIDDHARTA at DAΦNE, the proposed kaonic deuterium experiment will also measure the K-line transitions. The combination of both results allows the determination of the isospin-dependent ($I = 0, 1$) scattering lengths.

Since the yield for a kaon reaching the ground state is expected to be much lower for kaonic deuterium than for kaonic hydrogen, an upgrade of the SIDDHARTA-2 apparatus is essential, with the goal to increase the signal to background ratio by at least one order of magnitude. An important pillar of this upgrade was the development of the charged particle veto system, consisting of 96 plastic scintillators and silicon photomultipliers. First test measurements have been performed at the Stefan Meyer Institute. A time resolution of 51.5 ps and a detection efficiency of 99.3% were achieved for the veto-2 system.

FAKT SESSION III 14:00-15:30 THURSDAY, SEP 13

SR TDK

FAKT-11 TALK 14:00-14:25 THURSDAY, SEP 13

SR TDK

Lattice Fermions without Doubling

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Finite-difference schemes for the Dirac equation have long been plagued by fermion doubling: within the energy bands, the degeneracy on the lattice is higher than for the continuum Dirac equation, leading to counter-propagating “doublers”. In other words, the single cone of the continuum Dirac equation is mapped onto several cones on the lattice. We will first identify the origin

of fermion doubling and subsequently present a class of space-time staggered grids which avoid fermion doubling for the $(d+1)$ dimensional Dirac equation entirely: the single cone of the Dirac equation is mapped on a single cone of the lattice scheme. Specifically we will discuss numerical second-order accurate schemes for $d=2$ (topological insulator) and $d=3$ (high-energy physics) [1,2]. These schemes are explicit, of leap-frog type, and scale with the number of grid points. The single-cone energy dispersion will be demonstrated. Stability criteria, as well as the extension to mixed-state dynamics and to higher order lattice schemes will be discussed [3,4]. Time permitting, we will show examples for numerical simulations of Dirac fermion dynamics in electromagnetic textures in $(2+1)D$ [5].

- [1] R. Hammer et al, *J. Comp. Phys.* **265**, 50 (2014).
- [2] W. P., *Phys. Rev. E* **96**, 053312 (2017).
- [3] M. Schreilecher and W. P., *J. Comp. Phys.* **348**, 591(2017).
- [4] M. Schreilecher and W. P., *Comp. Phys. Comm.* **204**, 43 (2016).
- [5] W. P. And R. Hammer, *J. Appl. Phys.* **120**, 193903 (2016).

Funded in parts by FWF Austria.

FAKT-12 TALK 14:25-14:50 THURSDAY, SEP 13

HS TDK

Recent developments in the calculation of correlation functions of Yang-Mills theory

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Results for Yang-Mills correlation functions in the Landau gauge from equations of motion of 1PI and 3PI effective actions are reviewed. The status of the truncation dependence is discussed on the basis of results for nonprimitively divergent correlation functions and for the three-dimensional case. Special emphasis is put on the renormalization of the underlying equations and perturbative resummation.

FAKT-13 TALK 14:50-15:15 THURSDAY, SEP 13

SR TDK

Status of Hadron Structure Calculations in Continuum QCD

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The calculation of hadronic observables using a combination of Dyson-Schwinger and Bethe-Salpeter equations has developed dramatically in recent years. The method aims at the calculation of hadronic properties from the underlying QCD degrees of freedom, without abandoning the realm of continuum quantum field theories. We report on the most recent calculations of the spectrum and electromagnetic properties of baryons in this framework, highlighting the physical mechanisms that are currently included/excluded in those calculations.

Moreover, we outline the developments that will, foreseeably, take place in the near future, and how they will make the corresponding results reliable enough to be use as input for calculations in which hadronic information is needed.

On the dynamic generation of kinetic terms for mesonic bound states

Jordi París-López, Hèlios Sanchis-Alepuz, and Reinhard Alkofer

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Dynamical bosonisation within the functional renormalisation group is used to describe mesons as quark-antiquark bound states. Employing for simplicity the two-flavour quark-meson model it is exemplified how the kinetic terms for pseudoscalar and scalar mesons are generated from the quark kinetic term upon lowering the renormalisation group scale. Relating this method to the Dyson-Schwinger-Bethe-Salpeter approach one can identify the momentum-dependent Yukawa three-point function in the limit of vanishing renormalisation group scale with the Bethe-Salpeter amplitude. This in turn might allow for a systematic comparison of the impact of truncations in the Dyson-Schwinger-Bethe-Salpeter approach on the one hand and the functional renormalisation group with dynamical bosonisation on the other hand. This talk is concluded by an outlook on a respective on-going investigation.

FAKT SESSION IV 16:00-17:35 THURSDAY, SEP 13
SR TDK**The Size of the W-boson**

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Due to the fact that gauge variant states are no physical observable states, different approaches than perturbation theory have to be considered. We look at gauge-invariant composite operators and calculate two and three point functions using lattice technology. The considered operator consists of a W-boson-field dressed by two Higgs-boson-fields to obtain a gauge invariant vector operator. The results of the two and three point functions will be compared to perturbative results and will give an estimate for the validity of the Fröhlich-Morchio-Strocchi-mechanism. The three point function can then be used to calculate the size of the W-boson. The term “size” refers to the radius obtained from the first term of the Taylor expansion of the form-factor.

Mesonic bound states in a nearly-conformal gauge theory

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The matter content of a gauge theory is tuned such that one is close to the conformal window, but

still in the confining and chiral-symmetry-breaking regime. Properties of mesonic-type bound states are discussed. Preliminary results for the spectrum of such a theory are presented.

FAKT-17 TALK 16:30-16:45 THURSDAY, SEP 13

SR TDK

On the spectral dimensions seen by gluons

Wolfgang Kern, Markus Q. Huber and Reinhard Alkofer

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Based on the notion of the spectral dimension of a fractal we develop a tool to analyze the dynamics of gluons in three- and four-dimensional Yang-Mills theories in the Landau gauge. We detail the changes to a derivation of the spectral dimension from the diffusion of a hypothetical test particle which are needed so that this concept can be applied to fully dressed gluon propagators. The main result of our study is the fact the spectral dimension as seen by gluons drops from the topological dimension $d = 3$ resp. $d = 4$ for small diffusion times, resp. the ultraviolet, to two for long diffusion times, i. e. in the infrared. We comment on how this property might be related to gluon confinement.

FAKT-18 TALK 16:45-17:00 THURSDAY, SEP 13

SR TDK

On the quark-gluon vertex at nonvanishing temperature

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The phase diagram of Quantum chromodynamics (QCD) is expected to contain a plethora of interesting physics. However, a determination from first principle in the region of nonvanishing chemical potential region is currently unknown.

In this presentation, we use a complementary method to lattice simulation, the Dyson-Schwinger equations. The challenge, in this continuum approach, is to devise and solve an appropriate truncation of the corresponding equations. Here the application to theories similar to QCD but without the sign problem of lattice methods (QCD-like theories) becomes useful, as truncations can be tested by comparison to corresponding lattice results also at nonvanishing density.

The universality of a certain class of truncations is shown for three different theories including QCD. Going one step further, results for the quark-gluon vertex, the main model input of most contemporary studies, will be shown.

Pionic corrections to the mesons' quark core

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Within the rainbow-ladder truncation to the QCD Bethe-Salpeter equations the valence quark core of hadrons is described quite accurately. Calculated observables show, however, that so-called meson cloud corrections are missing. In this talk we will report on a systematic approach to include pionic corrections to the mesons' quark core.

On chiral perturbation theory for composite states

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Chiral perturbation theory is an effective field theory which treats chiral corrections to hadronic properties in a systematic way. Hereby, the bare hadronic states are treated as point-like objects. In this talk we report on an approach in which mesons are displayed as composite states described by their Bethe-Salpeter amplitudes. We will present preliminary results for the leading order chiral correction to selected mesonic properties.

The charged rotating mass shell and its gyromagnetic ratio in general relativity and modified gravity theories

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It has been claimed that relativistic, charged and rotating mass distributions possess a gyromagnetic ratio close to 2. We investigate this hypothesis by numerically solving the coupled Einstein-Maxwell equations for a charged rotating mass shell. An extension to modified gravity theories will be presented as well as preliminary results.

HISTORY of PHYSICS

(GEP)

GEP SESSION I 14:00-15:20 TUESDAY, SEP 11

SR TDK

GEP-1 TALK 14:00-14:40 TUESDAY, SEP 11

SR TDK

The life and science of Marie Curie and Lise Meitner - two icons of radioactivity

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In the year 2018 there are several anniversaries concerning Marie Curie and Lise Meitner: It is 120 years since the discovery of the new elements Polonium and Radium in Uranium ore by Marie and Pierre Curie (1898). Last year was also the 150th birthday of Marie Curie (*1867). This year is the 140th birthday of Lise Meitner (*1878) and it is 50 years since her death (1968). It is also 80 years since nuclear fission was radiochemically discovered by Otto Hahn and Fritz Strassmann toward the end of 1938 [1], and the physics of the fission process was explained by Lise Meitner and Otto Frisch in their exile in Sweden at about Christmas time that year [2,3].

Since both women are intimately connected with the development of radioactivity, an attempt will be made to describe their life and science in this presentation. Although scientifically both women were clearly outstanding, their personal life including the recognition of their scientific achievements could not have been more different. Marie Curie was born as Marja Skłodowska in Warsaw. In Paris she married Pierre Curie who also became her scientific partner. She won two Nobel Prizes (Physics 1903 and Chemistry 1911), had two daughters Irène and Ève, but lost her husband early on (1906) in a tragic street accident. Lise Meitner was born into a Jewish family in Vienna, left Vienna in 1907 and worked for 31 years in Berlin in close collaboration with the chemist Otto Hahn. In 1944 only Otto Hahn received the Nobel Prize in Chemistry “for his discovery of the fission of heavy nuclei”. None of the other players mentioned above was included. There exists an extensive literature on trying to understand the reasons for this injustice. Some of it will be summarized in the current presentation.

[1] O. Hahn, F. Strassmann, “Über den Nachweis und das Verhalten der bei der Bestrahlung des Urans mittels Neutronen entstehenden Erdalkalimetalle”, *Naturwissenschaften* **27**, Heft 1 (6 January 1939) 11-15.

[2] L. Meitner, O.R. Frisch, “Disintegration of Uranium by Neutrons: a New Type of Nuclear Reaction”, *Nature* **143**, issue 3615 (11 February 1939) 239-240,

[3] O.R. Frisch, “Physical Evidence for the Division of Heavy Nuclei under Neutron Bombardment”, *Nature* **143**, issue 3616 (18 February 1939) 276.

Double refraction on artful historical crystal slides and glasses with inner stressesPia-Felicitas Weinhart und Franz Sachslehner*Faculty of Physics, University of Vienna, Austria*

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Erasmus Bartholinus (1625 - 1698) discovered the phenomenon of double refraction on Iceland spar in 1669. Christian Huygens (1629-1695) introduced the split-up of light into an ordinary and extraordinary wave. The former propagates spherical, the latter ellipsoidal. Augustin Jean Fresnel (1788 - 1827) refined this idea for optically biaxial crystals. David Brewster (1781 - 1868) studied in great detail various phenomena with polarized light. In 1814 he also discovered stress double refraction on rapidly cooled glasses, as well as in an independent manner Johann Seebeck (1770-1831). In 1815, David Brewster found that even mechanical pressure on transparent bodies produced double refraction. As early as 1840, the scientific *PALMER'S NEW CATALOGUE* offered *unannealed glasses* and *selenite designs* (selenite is a variety of gypsum) to demonstrate double refraction.

The objects studied by us in experiment and theory correspond essentially to the design of the teaching aids, as can be found from 1840 and probably all the rest of the 19th century. Thus, the cork-framed gypsum preparations with motifs, as we still have them today, are in part already depicted in the catalogue of 1840, e.g. the *six-pointed star*, *ERIN GO BRAGH* or *DINNA FORGET*. Similarly, this applies to the unannealed glasses and glass presses. Our further samples, such as butterfly, *HEART'S EASE* and chameleon are mentioned at least in offer lists from 1851.

Both the gypsum preparations and the rapidly cooled or pressed glasses produce in the polarized light beautiful interference colours, which are in the bright field complementary to those in the dark field. The glasses with inner stresses show colourful isochromatics and, depending on the position of the analyser, black or white isoclinics which correlate with the geometric shape of the glasses.

From the 'Armarium' to the 'Institute of Experimental Physics' at the University of Innsbruck. The 275-year anniversary: 1743 - 2018

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An outline is given on nearly 350 years of history of Physics at the Universität in Innsbruck: 1st physics lecture 1670, 1st appointment of a Professor for Physics 1673, 1743 Ignaz von Weinhart, Professor of Mathematics, founded the so-called 'Armarium' - a small experimentation cabinet, up to the re-foundation of the University in the years 1945/1946. The 'Armarium', the nucleus of the Institute of Experimental Physics in Innsbruck, soon became an appreciated place of Natural History which, subsequently, contributed considerably to the development of the University: Under the guidance of Weinhart, his private student Peter Anich significantly contributed to cartography and land surveying, Joseph Stapf, Professor of applied mathematics and technology and Franz Zallinger, Professor of Physics, were the first to recognize the importance of teaching technical sciences, they were the pioneers of the 'Technical Faculty' founded in 1969. In 1868, due to the initiative of Adalbert Waltenhofen, the Institute of Mathematical Physics was implemented. 1867 Leopold Pfaundler, Privatdozent in physical chemistry, published his considerations on the application of kinetic theory to chemical reactions, and was appointed as Professor in Physics; this seminal paper

led to the posthumous ‘Chemical Breakthrough Award’ 2016 by the ‘American Chemical Society’. Due to the suggestion of Pfaundler, among others, a professorship for ‘Theoretical Astronomy’ was created in 1892, the basis and nucleus of nowadays ‘Astrophysics’. Both, Waltenhofen and Pfaundler, supported considerably the new and promising field of ‘Electrotechnics’, which led to the creation of the ‘Institute of Electrotechnics’ in 1907. In Addition, scientific work of Mache and Schweidler on radioactivity and atmospheric electricity, and of Victor Hess on the so called Ultrastrahlung led to the new field of ‘High-energy Physics’ in Innsbruck.

A considerable quantity of historical instruments prove the rich experimental history of Physics in Innsbruck. There are, among others: a conical mirror with related anamorphoses (1754), a Perpetuum Mobile (1817), triboluminescence tubes (1867), and, as highlights, an astronomical clock, donation of Empress Maria Theresia (1776), and geodetic instruments, donations of the bavarian King Maximilian I. Joseph (1807/08).

GEP SESSION II 16:00-17:20 TUESDAY, SEP 11

SR TDK

GEP-4 TALK 16:00-16:40 TUESDAY, SEP 11

SR TDK

Maxwell’s Demon: A Historical Puzzle with Impact on Modern Physics

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Maxwell’s demon brought to the scientific arena in 1871 still survives in modern physics. Invented as microscopic phantom to overrule the second law of thermodynamics as a way to gain illimitable energy from a heat reservoir without external intervention, he has been exorcised after recognizing its role in information theory (pioneering article of Leo Szilard 1929, bridging the gap between thermodynamics and information theory later introduced by C.E. Shannon 1949). The relation between “informal” and thermodynamic entropy and the cost of information storage/manipulation in computational sciences are answered by the pioneering works of R. Landauer (1961) and C.H. Bennett (1982) in the discovery of the “erasure principle”. However, is the demise of the demon still too early if quantum phenomena are brought into play? Quantum-mechanical versions of Maxwell’s demon exhibit features beyond classical versions: the microscopic system which produces “work” is closely linked (entangled) with the information produced by the quantum measurement and the heat bath acts as a source of decoherence. Szilard’s one-particle engine is extended to few more particles and revisited in terms of their indistinguishability and delocalization. Experimental verifications were long time out of realization (apart from “gedanken experiments”), but nanotechnology and manipulation of single atoms/spins has opened a way to investigate the thermodynamic microscopic “heat engine” cycle in detail.

The historical path from early suggested experiments (Smoluchowski’s ratchet, Brillouin’s rectifier) up to the most recent attempts (employing a trapped ultracold ion [1]), and the creation of the first photonic Maxwell’s demon [2] should elucidate the modern role of the less-than-fashionable “old” Maxwell’s phantom.

[1] L. L. Yan et al.: Single-Atom Demonstration of the Quantum Landauer Principle, *Phys. Rev. Lett.* **120**, 210601 (2018).

[2] M. D. Vidrighin et al.: Photonic Maxwell’s Demon, *Phys. Rev. Lett.* **116**, 050401 (2016)

Early Styrian Meteorological Records Revisited

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Written documentation of weather observation for the Graz region can be traced back to at least 1550, when the physician Petrus Widmann sporadically recorded them in his copy of an almanac. There is also some rumor that Johannes Kepler during his stay in Graz documented his daily weather observations, but no written proof in Kepler's handwritten scientific remains could be found (up to know). The next documented weather records originate from the Jesuit Karl Tierenberger (also Tirnberger), in a brief print published in Graz, 1770, summarizing his observations from 1765 to 1769 at the Graz astronomical observatory. The almost uninterrupted time series of meteorological measurements in Graz started in 1836 and were initiated by the professor of physics at Graz University, Julius Wilhelm Gintl (1804-1883).

Recently, we found out that there exists another time series of meteorological elements, which even predates the above measurements by about 44 years. Why this series fell into oblivion could not be figured out.

The time series starts with the year 1792 and lasts for more than 40 years. The instrumental readouts consist of atmospheric pressure and temperature measurements performed three times per day and of a remark to meteorography once per day. The measurements were taken in the inner city of Graz at the house of the family Rospini, who managed an optical workshop/manufacture and shop. The recordings were published in tabular form in the newspaper printed in Graz, namely the "Graetzer Mercurius", the "Graetzer Bürgerzeitung" and for the longest time period the "Graetzer Zeitung".

Additionally to the above mentioned measurements in Graz, we could also find a meteorological record for two entire years (mid 1819 to mid 1821) of another location in Styria, namely for Bärnegg in der Elsenau, in the Wechsel region. Franz Holler, son of the estate owner, former physics student at Graz University and graduate of the Klagenfurt agricultural school, documented the weather of this rather remote place in a handwritten manuscript, today kept in the Styrian Provincial Archive. He complemented the readout of his instruments by descriptive comments in his daily economic log.

Experimental Proof of Aetherdrift Disproves Hypothesis of Length-Contraction

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Recent detection of Aetherdrift as expected by Maxwell in 1879 proves that the length-contraction isn't element of physical reality. The method of measurement is based on Michelson's wave-theoretical discovery of the violation of the law of reflection published in the supplement of the historical paper on the interferometric attempt on Aetherdrift-measurement of Michelson and Morley in 1887.

PHYSICS and SCHOOL

(LHS)

LHS SESSION I 14:00-14:40 WEDNESDAY, SEP 12

HS P1

LHS-1 TALK 14:00-14:20 WEDNESDAY, SEP 12

HS P1

QUANT - Bringing current research to highschool physics education

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Physics is not very popular in highschool. Nevertheless, many people show a genuine interest in physics. For example, many know what a black hole is and have heard about “beaming” of photons. In the science communication project QUANT we want to give pupils the possibility to learn about things currently investigated at the University of Graz. To this end, topics are prepared for a webpage (quant.uni-graz.at) so that they can connect to the standard physics lessons in highschool. At the end of every module we give an overview of related research topics at the University of Graz. The topics range from particle physics to nanophysics to meteorology. The webpage also contains a forum and possibilities for the teachers to exchange experiences and teaching material.

LHS-2 TALK 14:20-14:40 WEDNESDAY, SEP 12

HS P1

The international physics students competition PLANCKS - Physics League Across Numerous Countries for Kick-Ass Students

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PLANCKS is a very exiting team competition for physics students from all over the world. Since its first realization in 2014, the number of participants has risen steadily. More than 30 teams from over 20 countries compete against each other in a four-hour competition. The teams of four students have to solve ten problems in four hours without any tools like books or computers. It is organized in national preliminary rounds, in which the best teams of each country compete for the tickets to the final round. PLANCKS is a unique experience for physics students from all around the world. It promotes international exchange, teamwork in solving problems and cultivates critical scientific discussions.¹

In 2017 the international final round took place in Graz where I (AP) was the vicepresident of the local organizing committee. I would like to present this unique competition to the audience, talk about the final in Graz and show ways how this great event can be promoted and supported in Austria in the future. In particular I would like to put a special emphasis on the Austrian preliminary

competition which is organized by the Austrian physics students' unions (ZöPV) every year around February and March.

[1] Dorn, G., Pflieger, A. J., Werl, M., & Arrigoni, E. (2018). PLANCKS 2017-Physics League Across Numerous Countries for Kick-Ass Students. *European Journal of Physics*.

MEDICAL PHYSICS, BIOPHYSICS and ENVIRONMENTAL PHYSICS

(MBU)

MBU SESSION I 14:00-15:30 THURSDAY, SEP 13

HS P2

MBU-1 TALK 14:00-14:15 THURSDAY, SEP 13

HS P2

X-ray Studies of Antimicrobial Peptide Activity in *E. coli* Inner and Outer Membrane Mimics

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Infectious diseases caused by multi-resistant pathogenic bacteria are rapidly gaining grounds world-wide. One highly promising strategy to combat infectious diseases is based on antimicrobial peptides (AMPs), effector molecules of innate immunity. We performed time-resolved X-ray scattering experiments on live *Escherichia coli* (*E. coli*) under the attack of AMPs. A preliminary global analysis in terms of a multi core-shell model [1] is highly encouraging, however, we need to further substantiate the obtained results at different levels of structural hierarchy. In order to get access to distinct structural information at the different length scales, the *E. coli* scattering intensity is dissected into different components, starting with lipid-only mimics of the inner (IM) and outer (OM) membrane as a bottom up approach.

As a mimic of the inner bacterial membrane we investigated large unilamellar lipid vesicles (LUVs) containing a mixture of phosphatidylethanolamine (PE) and phosphatidylglycerol (PG) to study the specific interactions of AMPs with IM lipids. Further, asymmetric LUVs (aLUVs) were investigated as a mimic of the OM. These vesicles contain a mixture of PE and PG on the inner leaflet of the lipid bilayer and lipopolysaccharides (LPS) on the outer leaflet, using a protocol recently developed by the Pabst group [2]. This enables us to learn about contributions of the IM and OM to the more complex systems of live *E. coli*, as well as specific interactions of the peptides with this lipid matrix. This will be further exploited to ultimately correlate time dependent changes on diverse levels of structural hierarchy in bacteria due to activity of AMPs.

[1] E. F. Semeraro et al. (2017). *IUCrJ* **4**(6)

[2] Eicher, B, et al. (2017). *J. Appl. Crystallogr.* **50**

Time-Resolved X-ray Studies of Antimicrobial Peptide Activity in Live *E. coli* on the Nano- to Micrometer Scales

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Novel antibiotics based on antimicrobial peptides (AMPs) are promising candidates for defending the spread of diseases caused by multi-resistant pathogenic bacteria. Some AMPs primarily interact with the cell wall, causing bacterial death by physically disrupting the barrier function of the cell envelope. Notwithstanding the number of works that explore the relationship between AMP activity and membrane architecture [1], the dynamics and full mechanism that lead to cell death are currently not clear. Here, we investigated the effect of different membrane-active peptides on live *E. coli* by means of high-resolution (Ultra) Small-angle X-ray Scattering (USAXS/SAXS) measurements performed on the ID02 beamline (ESRF, France).

Time-resolved USAXS/SAXS technique allowed to probe these systems in the appropriate length and time scales. Thanks to a very wide scattering vector (q) range, a multi-scale model provided valuable information about structural changes in both submicron and nanoscales (cell-body and cell-envelope, respectively) [2]. Results showed that key events occur on a few second, which is a time scale that was not previously accessible, and on a wide length scale, including electron-density variations in both cell-body and cell-envelope. In addition, the peptide-induced alterations of the bacterial structure exhibited well-defined time-evolutions which depended on the specific AMP. As an example, the mode of action of O-LF11-215 (derivative of the human lactoferricin) consisted of two distinct time regimes. Within the first 40 seconds, the structural parameters showed large-scale alterations (submicron range), possibly related to cell shrinking and loss of cytoplasmic content. At a later stage instead, results were addressed to a structural disintegration of the cell-envelope on the nanometer scale.

[1] G. Pabst and K. Lohner (2014). Membrane medicine. *In* Liposomes, Lipid Bilayers and Model membranes. From Basic Research to Application. G. Pabst, N. Kučerka, M.-P. Nieh and J. Katsaras, editors. CRC Press, Boca Raton, FL, pp. 217-245.

[2] E. F. Semeraro et al. (2017). *IUCrJ* **4**(6):751-757

IKOSA: Online Platform for Automated Image Analysis based on Artificial Intelligence

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In both academic and corporate research large numbers of diverse small-scale samples are repetitively investigated using different types of imaging modalities, e.g. microscopy. Due to ongoing digitization, digital images of the samples are usually present. However, the majority of them is

still analyzed manually and requires extensive expertise. These tasks are time-consuming, labor-intensive, and tedious, which results in long processing times, strongly subjective assessments, missing reproducibility, dependency on specifically trained staff, and high costs.

In order to solve these problems, KML VISION develops the IKOSA platform, a Software-as-a-Service (SaaS) to automatically and reliably analyze digital images. The platform consists of (a) specialized image analysis applications for e.g. counting or measuring objects, and (b) the IKOSA portal, where users can collaboratively manage data, trigger analyses and visualize results. The application portfolio is based on the most recent machine learning technology (Deep Learning), which is capable of solving very complex image analysis problems fully automatically.

The capability of IKOSA is demonstrated with one of the implemented applications: the automated detection of transcription factor (TF) activation in single living cells. These TFs that are labeled with an attached fluorescent protein shuttle between the cytosol and the nucleus of cells. Upon cellular stimulation of this transcription, specific TFs translocate into the nucleus to turn on genes to degrade and recycle cellular components in an ordered way. Large image datasets obtained with fluorescent microscopy have to be investigated to quantify precise time-dependent evaluation of transcription activation. Performance evaluations demonstrate that the results obtained with IKOSA are of same quality as manually obtained results. In addition, automated analysis is significantly faster to speed up research.

MBU-4 TALK 14:45-15:00 THURSDAY, SEP 13

HS P2

Calibration free measurement of optical force and torque of trapped particles

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Light carries energy and momentum, and thus exerts force and torque when interacting with matter, leading to a displacement and a rotation, respectively. By imaging the particle the force and torque strength can be determined, provided that the full force and torque landscape, or in a linear approximation, the trap stiffness matrix is known. A major difficulty of this approach is that this relationship between position/orientation and force/torque depends on a large number of parameters, which are often not well known or which are difficult to control accurately in an experiment.

In contrast to this approach, we present a direct way of measuring the optical force/torque acting on a particle based on the conservation of momentum by analyzing the far-field intensity distribution of the scattered light. This method has the great advantage that no information about size, shape or material of the particle is required, as it is the case for conventional methods. A central challenge in measuring optical torque is that the amplitude and phase are needed in order to calculate the angular momentum of the light. We present a phase retrieval approach which allows us to deduce the phase from a single intensity distribution measurement of the scattered light.

This project is funded by the Austrian Science Fund (FWF), Project P29936-N36.

Low-energy electron-induced decomposition of 5-trifluoromethanesulfonyl-uracil: a high-potential radiosensitizer

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Incorporation of halouracils into DNA enhances its radiosensitivity towards high-energy radiation. The reactivity of these compounds to low-energy electrons (LEEs) plays a crucial role in the sensitization process¹. The current gas-phase study assesses the propensity of a recently synthesized potential radiosensitizer, 5-trifluoromethanesulfonyl-uracil (OTfU), to dissociative electron attachment (DEA) in the electron energy range between $\sim 0 - 14$ eV. OTfU is a derivative of uracil substituted with a triflate (OTf) group at the C₅-position (see Fig. 1), which substantially increases its ability to undergo effective electron-induced dissociation². The measurements were carried out using a hemispherical electron monochromator coupled with a quadrupole mass spectrometer. We report a variety of fragments formed either by simple bond cleavages (e.g. dehydrogenation or formation of the triflate anion, OTf⁻) or by complex multi-bond rearrangements leading to a complete decomposition of the molecule. The most favorable DEA channel corresponds to the formation of the OTf⁻ as well as the reactive uracil-5-yl radical by the cleavage of the O–C₅ bond in uracil occurring mainly through a sharp resonance at 0 eV and other resonances (0.14, 1.05 and 3.65 eV) well below the threshold for electronic excitation. The dehydrogenated parent anion, (OTfU-H)⁻, is formed by the capture of electrons with energies below 2 eV. The latter reactions are mainly driven by the large electron affinity of the triflate anion (5.5 eV). Furthermore, the thermodynamic thresholds of the DEA reactions were predicted theoretically at the M06-2X/aug-cc-pvtz level both at the standard state and at a very low pressure of $3 \cdot 10^{-8}$ mbar to represent the experimental conditions. Ultimately, this study endorses OTfU as a potential radiosensitizing agent with further implications in tumor chemoradiotherapy.

JA, RM and FFS acknowledge the Portuguese National Funding Agency FCT-MCTES through grants PD/BD/114447/2016, PD/BD/114452/2016 and researcher position IF-FCT IF/00380/2014, respectively, and the research grant UID/FIS/00068/2013. The support from Polish National Science Center (NCN) under the Grant No. UMO-2014/14/A/ST4/00405 is also acknowledged (JR). This work was supported by Radiation Biology and Biophysics Doctoral Training Programme (RaBBiT, PD/00193/2012); UID/Multi/04378/2013 (UCIBIO). EAB and SD acknowledge support from FWF (P30332). Calculations have been carried out in Wrocław Center for Networking and Supercomputing (wcss.wroc.pl), grant No. 209.

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The effect of pressure on a liquid-liquid phase separated protein system induced by multivalent ions

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The understanding of protein interactions in aqueous solutions is crucial for many issues in soft and biology matter. A particularly interesting example for phase behavior in protein solution is the metastable liquid-liquid phase separation (LLPS). LLPS in protein solution is a fundamental biophysical phenomenon and provides a mechanism for biological structure and changes on the pathways of protein crystallization.

Because of the limited temperature range for protein solutions, pressure constitutes a key variable to achieve a complete description of the thermodynamic behavior of any protein solutions. The pressure window is much wider and goes up to several hundred MPa, before the proteins starts to denaturate.

We have shown that the interaction in protein solutions can be efficiently tuned by the variation of the ionic strength, the nature of the ions and the valency of ions. A rich phase behavior, including re-entrant condensation, metastable LLPS, cluster formation and crystallization has been observed when trivalent salts are used. A theoretical model was developed to describe these effects by proteins with attractive patches. LLPS can be observed when the attraction is sufficiently strong and the cation-induced hydration effects cause a lower critical solution temperature behavior in the studied system.

In this study we investigate the pressure dependent behavior of BSA under a LLPS. The diluted phases were collected and studied by SAXS. The strength of the interaction were calculated by using a sticky hard sphere model. The strength of the attraction varies with the pressure. At higher attractive strength the formation of aggregates can be observed. Pressure dependent NMR measurements showed no changes within the secondary structure of the protein within the applied pressure range. The combination of NMR and SAXS experiments shows that the equilibrium between monomers and dimers in BSA solutions is shifted to a higher monomer fraction at higher pressures.

SURFACES, INTERFACES and THIN LAYERS

(OGD)

OGD SESSION I 14:00-15:30 TUESDAY, SEP 11 **HS BE01**

OGD-1 TALK 14:00-14:30 TUESDAY, SEP 11 HS BE01

Surface Chemistry of 2D Materials

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Understanding the chemical reactivity of 2D materials such as graphene and hexagonal-boron nitride (h-BN) is of fundamental importance for obtaining flexible and tunable materials for devices and electronic applications, as well as for fundamental science to obtain concepts for the chemistry on such materials. The interaction of graphene and h-BN with oxygen and atomic hydrogen will be discussed in details and the results for the two substrates will be compared. While in the case of atomic hydrogen, graphene forms graphane, i.e. fully hydrogenated graphene, for h-BN hydrogen can bond and intercalate, depending on the exposure. Interestingly, graphene does not react with molecular oxygen, even when supplied with a high kinetic energy of 0.7 eV, while h-BN readily forms bonds to oxygen, intercalates or even reacts, depending on the substrate temperature. Further insights to the bonding and reaction mechanisms of hydrogen and oxygen are obtained from DFT calculations.

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OGD-2 TALK 14:30-14:45 TUESDAY, SEP 11 HS BE01

In₂O₃(111) – Surface Structure and Adsorption

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Indium oxide, In₂O₃, is the prototypical transparent conductive oxide, and is omnipresent in any application where electronic and optical properties are of essence. As the interface is central in all

these applications, understanding the fundamental properties is critical, especially when going to nanoscopic dimensions in novel device architectures.

As a model system we investigate the non-polar $\text{In}_2\text{O}_3(111)$ surface with low temperature STM/AFM, XPS and DFT, using single crystals. This talk gives an overview on our current investigations on $\text{In}_2\text{O}_3(111)$ including the adsorption of water and the interaction with the prototypical organic molecule sexiphenyl ($\text{C}_{36}\text{H}_{26}$, 6P).

Dissociative adsorption of water on the $\text{In}_2\text{O}_3(111)$ surface is observed above 100 K, where the dissociation takes place on lattice sites. At room temperature the surface is saturated with three dissociated water molecules per unit cell, symmetrically arranged around the six-fold coordinated In, In(6c) atoms. The fully hydroxylated surface shows a (1×1) structure with respect to the clean $\text{In}_2\text{O}_3(111)$ surface. The three terminal OH groups plus the three protons (forming surface OH groups) are imaged together as one bright triangle in STM. The internal structure is revealed by AFM measurements, and manipulations with the STM tip.

Surface science investigations have significantly contributed to understand the organics/metal interface, but the second electrode in such devices - the one that is optically transparent - is unknown territory. Our study closes this gap. We find that the 6P molecules adsorb in a flat lying and oriented geometry. From the adsorption site of the single molecules it is clear that the 6P prefers the interaction with the In(5c), and avoids the oxygen-terminated regions. At higher coverage the molecules reorient into a densely packed first monolayer with a distinct pattern that is also based on the atomic configuration: half the molecules are able to maintain their preference for adsorbing on In(5c) atoms.

OGD-3 TALK 14:45-15:00 TUESDAY, SEP 11

HS BE01

Surface phonon dispersion of $\text{Bi}_2\text{Se}_3(111)$: Surface Acoustic Waves and Charge Density Wave

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We present a combined experimental and theoretical study of the surface vibrational modes of the topological insulator Bi_2Se_3 [1]. Using inelastic helium atom scattering [2] we are able to resolve the acoustic and optical phonon modes of $\text{Bi}_2\text{Se}_3(111)$ up to energies of 18 meV. The low energy region of the surface phonons is mainly dominated by the Rayleigh mode which has been claimed to be absent in previous experimental studies [3]. On the other hand, the appearance of the Rayleigh mode is consistent with previous bulk lattice dynamics studies as well as theoretical predictions of the surface phonon modes [4,5]. However, our results do not support the presence of a Kohn anomaly, connected with a surface phonon mode, as inferred from a previous experimental study [3].

The speed of sound of the Rayleigh mode is determined to be between 1630 ms^{-1} and 1800 ms^{-1} from the experimental data depending on the crystal orientation. Comparison of the experimental data with the surface phonon dispersion as calculated by density functional perturbation theory shows excellent agreement. Moreover, there appear additional branches in the gap below the Rayleigh wave branch which cannot be attributed to any possible phonon branch of the ideal surface

based on the calculations. The recent observation of dynamical charge density wave excitations on the semimetal Sb(111) [6] as well as in cuprate superconductors [7] suggests the assignment of these additional low-energy excitations to phason-amplitudon pairs.

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OGD-4 TALK 15:00-15:15 TUESDAY, SEP 11

HS BE01

Influence of Substrate Temperature on Structural, Optical, and Electrical Properties of ZnO Deposited by Plasma-Enhanced Atomic Layer Deposition

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ZnO is a direct band gap semiconductor with attractive piezoelectrical, optical, and electrical properties, particularly appealing for a variety of functional devices (e.g., gas, bio, and UV sensors, piezoelectric nanogenerators and actuators). Being able to tailor these material properties to meet specific technological requirements is crucial for enhancing the device efficiency or sensitivity.

In a previous study [1], the effect of plasma power on plasma-enhanced atomic layer deposited (PE-ALD) ZnO had been investigated at room temperature. By tuning the power, several material properties had been tailored. However, the power had shown little influence on the texture of the crystalline films.

In this study, we investigated the effect of substrate temperature in the range 25°C - 250°C on the ZnO material properties. The films were grown by direct PE-ALD adapting diethylzinc and O₂-plasma as reactants. Atomic layer deposition is the method of choice for the growth of high-quality conformal films with Å-level thickness control. By adjusting the substrate temperature, it was possible to switch the texture of the films from (100) at room temperature to (002) above 150°C. The growth per cycle (obtained by spectroscopic ellipsometry, SE) ranged from 1.6 to 4.0 Å/cycle, suggesting a temperature dependent growth behavior. Further SE analysis showed a range of refractive index (at 633 nm) from 1.87 to 1.94 and a bandgap range of 3.255 to 3.270 eV. X-ray photoelectron spectroscopy survey scans pointed out a non-detectable carbon content and a O/Zn ratio of around 1.17 (constant over the whole temperature range), while high-resolution scans of the O1s-peak showed a decrease in OH-content from 21% (at 25°C) to 9% (at 250°C). Further analysis will focus on resistivity (and its relation to OH-content), transparency, and piezoresponse.

Correlating the results of these techniques, interesting insights can be gained into the quality of the PE-ALD ZnO and which substrate temperature should be chosen for specific applications. This paves the way for optical, electrical, or sensing devices on the basis of tailored ZnO thin films, which can be grown conformally and with Å-level thickness control due to the PE-ALD characteristics.

- [1] Pilz *et al.*, *J. Vac. Sci. Technol. A* **36.1** (2018): 01A109.

Initial ZnO Crystallite Formation by Plasma Enhanced Atomic Layer Deposition

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ZnO is a wide direct bandgap semiconductor, extensively studied as thin film because of its unique opto-electrical properties. Its crystalline structure has a crucial impact on the material characteristics and its applicability in opto-electronic devices. Therefore, control over the preferred crystallographic orientation in ZnO thin films has been often investigated.

Atomic layer deposition (ALD) is a self-limiting deposition method, mainly adopted for the delivery of (ultra-)thin films. Due to its layer-by-layer nature, details on the nucleation and growth of materials can be investigated. Next to ALD, plasma enhanced ALD (PE-ALD) is an alternative method which employs reactive plasma as co-reactant. Thin films deposited with PE-ALD show several differences when compared to ALD, such as different textures and lower defect formation. Therefore, for ZnO thin films the growth mechanism and initial crystallite formation may be greatly influenced by the use of plasma when compared to classical ALD.

In this contribution, the initial growth of direct PE-ALD ZnO grown on Si (100) is investigated. DEZ and pure oxygen plasma are adopted during the process. The first stages of growth are analysed using synchrotron light grazing incidence X-ray diffraction (GIXD), X-ray reflectivity (XRR), and spectroscopic ellipsometry (SE). The influence of substrate temperature (25°C to 250°C) on the crystal growth and orientation are studied. A closed layer was obtained within 7 cycles for all the temperature explored, suggesting island growth of the ZnO. However, GIXD showed no crystalline texture at this stage. An amorphous intermixed interface between the native SiO₂ and the growing layer was found, with a density in between pure SiO₂ and ZnO. Irrespective of the deposition temperature, the first crystal structure was measured at around 3 nm, with a preferential out-of-plane orientation transitioning from (100) to (002).

OGD SESSION II 16:00-17:30 TUESDAY, SEP 11**HS BE01**

OGD-6 TALK 16:00-16:15 TUESDAY, SEP 11

HS BE01

Transition Metal Clusters on Zirconia (ZrO₂) Thin Films: Growth and Metal-Oxide Interactions

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Zirconia (ZrO₂) is widely used in heterogeneous catalysis, gas sensors and solid oxide fuel cells, where it is interfaced to transition metals. However, most investigations of ZrO₂/metal systems focus on powder samples, where surface-science techniques of high spatial (e.g. scanning tunneling microscopy (STM)) or energetic (e.g. x-ray photoemission spectroscopy (XPS)) resolution are hampered by the morphology and insulating nature of the samples.

We have developed a method to prepare clean, atomically flat ZrO₂ films (5-6 O-Zr-O trilayers) by sputter deposition on Rh(111) [1]. Using different annealing temperatures, we can achieve a precise

control of the crystallographic phase of the ZrO₂ films (tetragonal or monoclinic). The films are thin enough for STM and XPS measurements, yet show bulk-like crystallography. Transition metal (Ni, Fe, Rh, Au, Ag) clusters were deposited on both phases of ZrO₂. The metal clusters show different morphology and density compared with those on ultrathin zirconia films (single trilayer) [2]. This indicates different interaction with the ZrO₂ surface. The metal-ZrO₂ interaction is also reflected in XPS core-level shifts of the ZrO₂ signal after metal deposition. Among the metals deposited, Ag has the weakest interaction with the substrates, and Ni, Fe the strongest. On tetragonal ZrO₂ films, XPS shows small shifts of the Zr 3d and O 1s core-level peaks upon metal deposition; the core levels shift much more on monoclinic films. This can be explained by the electronic structures of these ZrO₂ phases. Our work indicates the possibility of tailoring the properties of transition metal clusters by the thickness and crystallography of the oxide support and will shed light on the interfacial interactions in zirconia-supported catalysts.

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OGD-7 TALK 16:15-16:30 TUESDAY, SEP 11

HS BE01

Wet chemical preparation of CeO₂(111) supported Au catalyst

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Liquid phase deposition (LPD) is the most common way to produce heterogeneous catalysts in industry. For this purpose, a metal oxide powder is stirred in a solution containing a noble metal precursor. In an ideal case, uniformly distributed metal nanoparticles are supported on the metal oxide after rinsing, drying and calcination. Despite its broad application, the microscopic development of this process is poorly understood. Only few studies examined the LPD of gold on defect-free single crystal metal oxides [1,2]. For the first time, this work characterises the Au/CeO₂(111) model catalyst after each step of the wet chemical catalyst preparation. Chemical composition, cluster size and distribution are determined *ex situ* by surface science methods.

We will discuss the influence of LPD specific parameters such as solution pH, rinsing, and calcination on the oxidation state and cluster morphology of the gold nanoclusters. This has been determined in UHV by XPS, STM and TPD. We have found that Au¹⁺ and Au³⁺ species are the main compounds that adsorb to the partially hydroxylated CeO₂ surface indicating a grafting reaction as it was proposed on TiO₂, Fe₂O₃, and Al₂O₃ before [1,3]. After rinsing chloride has been completely removed and gold species have been reduced. Former studies on Fe₃O₄ and other metal oxides have shown that gold has been completely reduced to Au⁰ after rinsing and annealing [2,4]. In contrast, we have observed that a small part of the Au¹⁺ species remains on Ceria, even after annealing at 600 K. The amount of the Au¹⁺ species seems to depend on the precursor solution pH and the reduction degree of the supporting CeO_x(111).

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To be or not to be alloyed: The unexpected behaviour of Ni-Au and Co-Au core-shell nanoparticles upon heating

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We present transmission electron microscopy (TEM) studies of 5 nm Ni-Au and Co-Au core-shell particles on heatable TEM grids. The bimetallic nanoparticles, grown fully inert within superfluid helium nanodroplets, are monitored through a heating cycle from room temperature up to 1000°C. A new image processing method is presented, which allows the measurement of the temperature dependent diffusion constant at the nanoscale.[1] Particularly interesting are studies of oxidation effects and structural rearrangements in core-shell systems where a reactive metal (e.g. Ni) is covered by protective layers of a Au shell. The mere presence of oxygen species during TEM measurements enhances the process of Ni diffusion through the Au shell.[2] The structural integrity of ferromagnetic cores under gas atmosphere plays an important role for future applications of these novel bimetallic nanoparticles.

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Thermally induced alloying process in core@shell AgAu particles: A new method to measure diffusion on the nanoscale

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Core@shell nanostructures are a promising class of materials with outstanding physical properties and distinct fine-tuning possibilities with respect to size, morphology and the variety of composition. In the presented study we utilized superfluid helium nanodroplets, an ultra-cold and perturbation free matrix, to synthesise Au@Ag and Ag@Au clusters. After deposition onto a heatable transmission electron microscopy (TEM) grid, the clusters were monitored during a heating cycle from room temperature to 600 K. Using high resolution TEM with atomic resolution we can hereupon determine the composition and morphology of the clusters during the heating cycle. The core@shell structures begin to soften at higher temperatures and the clusters are fully alloyed at temperatures below 600 K. This alloying process is studied for Au@Ag and Ag@Au structures < 5 nm with a new image-processing method, which allows determining the temperature depended diffusion constant for finite systems. This first quantification of this process sheds light on the thermodynamic properties of nanometre systems and provides new input for current theoretical studies.

Helium Nanodroplet Based Synthesis of Tailored Nanoparticles for Surface Enhanced Raman Spectroscopy

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Nano-sized metal structures composed of bimetallic nanoparticles are attracting increasing interest due their tailorable properties, thereby opening new prospects for plasmonics and catalysis. We introduce the helium nanodroplet synthesis approach as a novel and versatile method for the production of functional nanostructures, assembled by the deposition of nanoparticles formed in the inert low-temperature helium environment.

For Ag@Au core@shell nanoparticles [1] deposited on fused silica substrates we present an investigation of the dependence of the localized surface plasmon resonance (LSPR) on the relative Ag:Au ratio using UV-vis absorption spectroscopy. The LSPR shifts from blue to red with increasing Au doping level, which can be conveniently controlled. [2] We further show that the nanostructures formed by the deposition of Ag@Au particles can be employed for surface enhanced Raman spectroscopy (SERS). Raman spectra for Ag@Au nanoparticles functionalized with 4-Methylbenzenethiol have been recorded, the enhancement for three different Raman laser wavelengths agrees well with the observed position of the LSPR peak and decreases with increasing Au content.

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Plasmon spectroscopy of metallic nanoparticles on ultra-thin h-BN films

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Ultra-thin hexagonal boron nitride (h-BN) films are employed as substrates for scanning transmission electron microscopy (STEM). The thickness of only a few atomic monolayers, the flat surface, and the relatively large bandgap of 5.97 eV [1] provide a unique set of properties, which makes h-BN ideally suited for high resolution plasmon spectroscopy by means of electron energy loss spectroscopy (EELS) [2]. The produced h-BN films have been placed on a holey carbon support and have an average thickness in the range of only 1 nm (~0.32 nm per monolayer [3]). H-BN is a superior substrate regarding the signal-to-noise ratio of the acquired EELS signal and the zero-loss peak (ZLP) width.

We present results on the investigation of plasmon modes of Ag, Au, and Ag@Au core@shell nanoparticles which lie in the transparent energy range of the h-BN substrates [4]. The particles were

fabricated utilizing the helium nanodroplet synthesis approach [5], allowing for a surfactant free production of tailored structures. Plasmon spectroscopy with EELS has the advantage of providing access to spectrally and energetically resolved plasmon resonance maps.

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OGD SESSION III 14:00-15:30 WEDNESDAY, SEP 12

HS BE01

OGD-12 TALK 14:00-14:30 WEDNESDAY, SEP 12

HS BE01

Dielectric interlayers: Promoters of charge transfer or inert decoupling layers or both?

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Recently we have shown that thin dielectric layers can actively promote charge transfer from the underlying metal substrate to molecules adsorbed on them [1]. Here a comprehensive analysis of the phenomenon of charge transfer promoted by a dielectric interlayers will be attempted principally using pentacene on MgO films of controlled thickness and work function. Imaging the orbitals in real and reciprocal space, with scanning tunneling microscopy and valence band photoemission tomography, supported by density functional calculations, we are able to unambiguously identify the orbitals involved and quantify the degree of charge transfer. Our experimental approach allows a direct access to the individual factors governing the energy level alignment and charge transfer processes for molecular adsorbates on dielectrics. Here the role of the work function, electron affinity, polarizability and dielectric thickness, is explored. Questions addressed will include: how is the work function catastrophe avoided, when and how is Fermi level alignment achieved and why has the phenomena not been observed in the past?

[1] M. Hollerer *et al.*, *ACS Nano* **11**, 6252 (2017)

OGD-13 TALK 14:30-14:45 WEDNESDAY, SEP 12

HS BE01

Photoemission Tomography of NiTPP on Cu(100)

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In this work we present a comprehensive characterization of the geometrical and electronic structure

of self assembled Nickel-tetraphenylporphyrin (NiTPP) films on Cu(100) utilizing various experimental techniques, supported by theoretical calculations using density functional theory (DFT). In particular we make use of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and photoemission tomography (PT), where the results of angle resolved photoemission spectroscopy (ARPES) measurements are systematically compared to the Fourier Transform of molecular orbitals, obtained in DFT. On the basis of STM and LEED measurements, we find, that NiTPP can arrange in two different geometrical configurations. In terms of electronic structure, PT allows for a direct assignment of peaks in the angle integrated ARPES spectrum to individual molecular orbitals and as such we observe a strong interaction of NiTPP with the metallic substrate resulting in occupation of LUMO/LUMO+1 and the LUMO+3 of the gas phase molecule. Our work emphasizes that a multi technique approach is essential in order to have a complete picture of the adsorption behavior and electronic properties of the metal/molecule interface.

OGD-14 TALK 14:45-15:00 WEDNESDAY, SEP 12

HS BE01

Ab-initio Structure Prediction of TCNE on Cu(111): From Monolayers towards Thin Films

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In presence of a surface organic molecules often crystallize in special phases with properties superior to those of bulk phases. However, resolving those surface-induced thin film phases remains a huge challenge, in particular for first-principle calculations. While efficient structure determination strategies exist for the adsorption of isolated molecules and to a limited extend also for molecular monolayers, none of these are efficiently applicable to organic thin films.

In this contribution, we demonstrate a strategy to bridge this gap with the SAMPLE^{1,2} approach: By combining single molecule adsorption geometries we first create an exhaustive set of monolayer structures. We then choose a small subset of these structures using experimental design (D-optimality criterion) and calculate their adsorption energies using dispersion-corrected density functional theory (DFT). Based on these adsorption energies we apply Bayesian linear regression to find an energetically optimized first adsorbate layer as well as the phase diagram for this layer. In order to predict multilayer structures we then consider this first layer as new surface on which a second layer adsorbes.

Here we use this approach to predict phases of TCNE (tetracyanoethene) adsorbed on Cu(111) at various coverages. For this system, we found that structures consisting of face-on geometries are energetically favorable at low coverage. We then investigate whether at increasing coverage a phase transition to densely packed, upright standing molecules occurs, or whether - and in which structure - a TCNE bilayer forms.

[1] V. Obersteiner, M. Scherbela, L. Hörmann, D. Wegner, and O. T. Hofmann, *Nano Lett.* **17** (7), pp 4453-4460 (2017)

[2] M. Scherbela, L. Hörmann, A. Jeindl, V. Obersteiner, and O. T. Hofmann, *Phys. Rev. Materials* **2** (4), 043803 (2018)

Crystalline growth of flexible organic molecules: 6P on Ag(001)

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Understanding the crystalline growth and energetic alignment of organic molecules on potential electrode substrates is crucial for the development of new and improved organic electronic devices. Within this work, we study the adsorption behavior of the organic molecule para-sexiphenyl (6P) on a single crystalline Ag(001) substrate in ultra-high vacuum conditions. Combining a series of surface-science techniques (STM, LEED, TPD, UPS) as well as theoretical calculations (DFT) we study the molecular film-growth of the isolated molecule up to the saturated wetting layer. The so obtained results are then related to SFM and XRD measurements of 6P bulk of *in-situ* grown thick films. Starting with the dilute monolayer, we observe the development of three phases with increasing film thicknesses, including molecular realignments, until the wetting-layer is saturated. We find that the complex molecular film development results from increasing intermolecular interactions, facilitated by the intramolecular twisting of the phenyl-rings. Furthermore, we observe no charge transfer to the molecule, indicating a weak molecule-substrate interaction of solely physisorbed nature. Finally, we characterize the complex bilayer-phase, which we can identify as the actual template for the development of device-relevant macroscopic organic crystallites.

Taming the Configurational Explosion: Coarse Grained Modeling and Statistical Learning for Surface Structure Search

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Monolayers of organic molecules on inorganic substrates often show rich polymorphism with diverse structures in differently shaped unit cells. Determining the different commensurate structures from first principles is far from trivial due to the large number of possible polymorphs. We introduce the SAMPLE approach^{1,2}, which employs coarse-grained modeling in combination with Bayesian linear regression to efficiently map the entire the potential energy surface and ab initio thermodynamics to generate phase diagrams.

To this end, we first determine adsorption geometries, which isolated molecules adopt on the substrate. Secondly, we generate all possible unique substrate super cells, whose area lies within predefined boundaries. Thirdly, we combine the local adsorption geometries with each super cell to generate possible structures. For two different subsets of these structures, we calculate the adsorption energies using dispersion-corrected density functional theory (DFT). The first subset serves as training data for a Bayesian linear regression algorithm, which allows to predict the adsorption energies of all possible polymorphs. The second subset allows us to validate the prediction. Finally, we employ ab initio thermodynamics, which assumes that the adsorbed layer is in thermodynamic equilibrium with an ideal molecule gas, to generate phase diagrams.

We demonstrate the power of SAMPLE on the system of naphthalene on Cu(111). For this system

we predict the adsorption energies for a large number of structures and determine the phase diagram.

[1] V. Obersteiner, M. Scherbela, L. Hörmann, D. Wegner and O. T. Hofmann, *Nano Lett.* **17** (7), pp 4453-4460 (2017)

[2] M. Scherbela, L. Hörmann, A. Jeindl, V. Obersteiner and O. T. Hofmann, *Phys. Rev. Materials* **2** (4), 043803 (2018)

OGD SESSION IV 16:00-17:30 WEDNESDAY, SEP 12

HS BE01

OGD-17 TALK 16:00-16:30 WEDNESDAY, SEP 12

HS BE01

Porphyrin Adsorption at Metal Oxide Nanoparticle Surfaces and Solid-Liquid Interfaces

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The efficient functionalization of metal oxide nanostructures with organic and metal-organic dyes is a prerequisite to realize hybrid materials for photosensitization, for electrochemical sensors or for molecular switches. The preparation of these materials is typically performed in the liquid phase, where an immobilized particle system is immersed into a solution containing the functional molecule. Herby the ubiquitous presence of water in the surrounding atmosphere and as an impurity in the solvent can have a significant impact on the adsorption mechanism and consecutive surface reactions and therefore for the efficient functionality of the device.

We investigated the adsorption of 2H-Tetraphenylporphyrin (2HTPP) with vapor phase grown MgO and TiO₂ nanoparticle systems. Porphyrin adsorption and subsequent metalation reactions were achieved under high vacuum conditions as well as in organic solvents. Vis diffuse reflectance and photoluminescence emission spectroscopy provide clear evidence for the promotion of interfacial reorganization processes of the adsorbate species by coadsorbed solvent molecules in liquids. Moreover, traces of spurious water were found to induce protonation-deprotonation reactions on the adsorbed porphyrins with a strong impact on the optical properties of the resulting hybrid materials.

OGD-18 TALK 16:30-16:45 WEDNESDAY, SEP 12

HS BE01

Metalation of Organic Molecules: Tetraphenylporphyrin on thin films MgO(001)/Ag(001)

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The metalation of free-base tetraphenyl porphyrin (2H-TPP) on various metal surfaces has been extensively studied in the literature due to their potential in a variety of future technologies. On most metal surfaces, porphyrins and metalloporphyrins adsorb in a flat adsorption geometry and form a square superstructure by self-assembly at/or above room temperature. Much less investigated is the adsorption and metalation of porphyrins on oxide surfaces. However, metalation of 2H-TPP has

been reported, e.g., on MgO [1,2] and TiO₂ [3]. Here, we present a comprehensive investigation of the adsorption and metalation of 2H-TPP on Ag(001) and MgO(001)/Ag(001) using LEED, TPD, STM, XPS and UPS. While the molecule adsorbs unmodified on the bare Ag(001) substrate, metalation of 2H-TPP on the MgO(001)/Ag(001) substrate is confirmed. We demonstrate that metalation of the 2H-TPP on Ag(100) can also be achieved by dosing with atomic Mg. Furthermore, we analyse the film-growth and electronic structure for both the unmetalated and metalated molecules. Of particular interest is, for both metalated monolayers, a hitherto unreported molecular state nearly 1 eV below the Fermi level. This new state will be discussed in terms of a singly charged molecular orbital.

[1] J. Schneider *et al.*, *ACS Appl. Mater. Interfaces* **7** (2015) 22962.

[2] J. Schneider *et al.*, *Chem.-Eur. J.* **22** (2016) 2744.

[3] J. Köbl *et al.*, *ChemistrySelect* **1** (2016) 1744.

OGD-19 TALK 16:45-17:00 WEDNESDAY, SEP 12

HS BE01

Electronic states of porphyrins at surfaces: the signature of supramolecular network formation

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Porphyrins are a family of aromatic molecules that gathers a strong community interest due to highly promising and successful surface applications, such as surface catalysis, lighting and energy harvesting. In applications, organic-inorganic structures with a few to several monolayer thick porphyrins films are utilized. Successful functionalization depends on the alignment of the porphyrin levels with the substrate. Investigation by state of the art spectroscopy techniques reveal porphyrin-related HOMO and LUMO peaks and a HOMO-LUMO gap that cannot be satisfactorily explained by the common model of a standalone or adsorbed porphyrin. In order to unravel the nature of these features, we investigate supramolecular networks and film formation, and its influence on electronic and photophysical properties. The thickness of such films allows models based on e.g. experimentally reported crystal phase. Here we focus on H₂TPP and MgTPP. Since these porphyrins possess large macrocycle and aromatic character, strong dispersive interactions arise. We use VdW-DFT for obtaining the structural properties, and many-body perturbation theory within the sc-qpGW-approach (calibrated against NIST data) for calculating the electronic spectra. The film formation involves a competition between the solvent energy and energy of formation. Our *ab initio* calculations, and other work in the literature suggest that the surface adsorption energy tends to be very close to film formation energy, thus, depending on the substrate, film formation or agglomeration of porphyrins are likely. A thick film leads to a considerable decrease in the HOMO-LUMO gap compared to the standalone molecule and also a non-symmetric peak broadening distinct from thermal broadening due to dispersion of the bands. The calculated HOMO-LUMO gap and the level-position agrees with the features seen UPS/2PPE spectra. Our findings underline that the formation of films or supra molecular networks has important influence on the electronic levels.

Interfacial band engineering of MoS₂/gold interfaces using pyrimidine containing self-assembled monolayers

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This study aims at finding strategies for avoiding the high contact resistance between gold electrodes and the two-dimensional semiconductor molybdenum disulfide. We demonstrate that tuning the work function (WF) of gold by pyrimidine-containing self-assembled monolayers (SAMs) can be used to eliminate the high injection barrier at the interface between gold electrodes and molybdenum disulfide thin films.

Exfoliated single-crystalline flakes of MoS₂ with 5-15 mono-layer thickness have been used in this study. The flakes were transferred onto pre-fabricated substrates suitable for the fabrication of field effect transistors (FET) comprising SAM functionalized gold electrodes that act as bottom contacts for MoS₂. Through combining the electrical characterization of the MoS₂-based FETs with various SAM treated electrodes, with modelling the devices characteristics, and Kelvin probe force microscopy investigations of the devices during operation, the strong influence of the injection barrier on the device performance is revealed.

In cases, where the SAMs induce a suitable alignment of the transport levels of the semiconductor flakes with the WF of the electrodes, the contact resistance becomes irrelevant and intrinsic properties of MoS₂ become accessible. In contrast, high injection barriers lead to a sizable contact resistance, and almost the entire bias voltage drops at the contact. As a consequence, the device performance is deteriorated and the drain current drops by several orders of magnitude.

Controlling initial stages of organic thin film growth by the step width of ion beam modified TiO₂(110)

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Due to its atomic rows in [001] direction the rutile, TiO₂(110) surface represents a highly anisotropic template for organic thin film growth. [1] This substrate can be further manipulated using ion bombardment under oblique angles yielding nanometer size ripple structures that influence the morphology and stability of para-hexaphenyl (6P) thin films. [2, 3] Depending on the projected ion beam direction, nanometer size ripples in either [001] direction parallel to the atomic rows or perpendicular to them in [1-10] direction can be created. The ripples remain crystalline and exhibit short (110) terraces separated by atomic steps as confirmed by low energy diffraction (LEED) and scanning probe microscopy (SPM). Depending on the terrace width, which can be well adjusted by the ion bombardment parameters, the 6P film properties can be tuned. Terraces, sufficiently large

can accommodate flat lying 6P molecules promoting needle like growth whereas on steep ripples with short terrace width only islands of upright standing molecules can exist.

[1] D. Wrana, M. Kratzer, K. Szajna, M. Nikiel, B. R. Jany, M. Korzekwa, C. Teichert, F. Krok, *J. Phys. Chem C* **119**, 17004 (2015).

[2] M. Kratzer, D. Wrana, K. Szajna, , F. Krok, C. Teichert, *PCCP* **16**, 26112 (2014).

[3] K. Szajna, M. Kratzer, D. Wrana, C. Mennucci, B. R. Jany, F. Buatier de Mongeot, C. Teichert, F. Krok, *J. Chem. Phys.* **145**, 144703 (2016).

OGD SESSION V 14:00-15:30 THURSDAY, SEP 13

HS BE01

OGD-22 TALK 14:00-14:15 THURSDAY, SEP 13

HS BE01

Rotation and Translation of a Single Molecular Dipole

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Controlling matter on the atomic scale using the tip of a scanning tunneling microscope (STM) is now a well-established field. The *pushing* and *pulling* STM manipulations employ rather close-range interactions and can be used to position single atoms and molecules on a surface with exquisite precision. Furthermore, a number of molecular processes such as rotation and conformational switching can be induced through inelastic electron tunneling or through interaction with the electric field in the STM junction. However, gaining control over the *direction* of rotation and translation of single molecules is more challenging. In the current work it is shown that an in-built permanent molecular dipole can be used to achieve a high degree of control over the motion of a single molecule. Through interaction of this dipole with the electric field of the tip, unidirectional rotation and translation is demonstrated [1]. Additionally, by mapping the behaviour of this motion, it is possible to visualize the internal electric dipole in a single molecule.

[1] G. J. Simpson, V. García-López, P. Petermeier, L. Grill, and J. M. Tour, *Nat. Nanotechnol.* **12** (2017) 604.

OGD-23 TALK 14:15-14:30 THURSDAY, SEP 13

HS BE01

Corroborating diffusion mechanisms between cryogenic and ambient temperatures

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We present a study of the diffusion of the organic molecule cobalt phthalocyanine (CoPc, $C_{32}H_{16}CoN_8$) on a Ag(001) substrate. The family of phthalocyanine molecules is used for active layers in electronic devices such as organic solar cells and organic field emission transistors[1] and CoPc has recently also been utilised as a single molecular magnet with possible applications in spintronics and quantum computing[2,3].

We show that by combination of two experimental techniques, helium spin-echo (HeSE) spectroscopy[4] and scanning tunneling microscopy (STM)[5], it is possible to obtain a complete picture of the diffusion of these molecules over the entire temperature range, from the onset of diffusion to technologically relevant temperatures. While STM is capable of providing information in the low temperature regime, HeSE can be used to get a better insight in diffusion at higher temperatures as well as at high coverages. It allows to elucidate a complex diffusion mechanism which includes steering through a metastable state and adsorbate interactions: With increasing temperature the activation of a metastable adsorption state occurs with the molecule in a different rotation and at a larger distance to the surface.

The presented approach promises to provide a route by which the factors affecting the underlying structural assembly in organic thin films can be explored and understood at a molecular level.

[1] O. A. Melville *et al.* *ACS Appl. Mater. Interfaces* **7**, 13105 (2015).

[2] M. Warner, M *et al.*, *Nature* **503**, 504 (2013).

[3] K. Bader, *et al.*, *Chem. Commun.* **52**, 3623 (2016).

[4] A. Tamtögl *et al.*, *Nanoscale* accepted (2018).

[5] G. Antczak *et al.* *JACS* **137** 14920 (2015).

OGD-24 TALK 14:30-14:45 THURSDAY, SEP 13

HS BE01

Selective dissociation of intramolecular bonds by STM manipulation

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Manipulation of molecules adsorbed at surfaces is very appealing to control and understand fundamental chemical processes. Chemical reactions can be triggered in single molecules by using the energy of the tunnelling electrons in a scanning tunnelling microscope (STM). Specifically, chemical bonds within molecules can be cleaved [1], the resulting fragments can be pulled across the surface by lateral manipulation with the STM tip and even new bonds can be formed [2].

In this work, we study the dissociation of single Br atoms from dibromoterfluorene (DBTF) molecules adsorbed on the Ag(111) surface. Experiments were done with a low temperature STM and applying voltage pulses where the Br substituents are located. By studying the current signal during the voltage pulse as well as imaging the single molecule before and after such a manipulation, we obtain insight into the process. After dissociation, single Br atoms and the remaining molecule are laterally dislocated over the surface, which reveals details about the interatomic interactions.

[1] B. C. Stipe, M. A. Rezaei, W. Ho, S. Gao, M. Persson, and B. I. Lundqvist, *Phys. Rev. Lett.* **78**, 4410 (1997)

[2] S.-W. Hla, L. Bartels, G. Meyer, and K.-H. Rieder, *Phys. Rev. Lett.* **85**, 2777 (2000)

Aggregation of Metallophilic Molecules on Surfaces

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Metallophilicity describes attractive interactions between two or more metal atoms with closed shell configurations (i.e. d^8 , d^{10}). Metal complexes containing gold in the formal oxidation state +I exhibit a very strong attractive interaction, which is also referred to as aurophilicity [1]. This type of interaction determines often the arrangement of gold(I) complexes in the solid state. However, there are almost no examples in literature, where this attractive interaction was studied on surfaces.

This experimental study focuses on the investigation of 2-naphthyl-isonitrile-gold(I)-chloride on Au(111) surfaces. This molecule is stable enough to sublime under ultrahigh vacuum conditions at moderate temperatures of 400 K. Ultrathin films of this organic material were prepared by physical vapor deposition on a Au(111) crystal. The deposition was monitored by differential reflectance spectroscopy (DRS) and photoelectron emission microscopy (PEEM). The transient of the mean electron yield, which was deduced from the sequence of the PEEM images, is strongly affected by the amount of molecules on the substrate. The evolution of the electron yield can be related to the change of the work function. In addition, the structure of the organic film was analyzed by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) confirming the presence of homodimers, similar to those of the bulk structure [2]. The dimers exhibit a crossed-swords arrangement with the gold atoms at the center of the cross indicating the aurophilic interaction between the two molecules forming the dimer.

[1] P. Pyykkö *et al.*, *Chem. Rev.* **97**, 597 (1997).

[2] E. Hobbollahi *et al.*, *Inorg. Chem. Commun.* **65**, 24-27 (2016)

Reversible Switching of Azobenzene Tetramers Molecules on a Metal Surface

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Molecular switches revealing reversible isomerization properties are potentially relevant building blocks in the fields of molecular electronics, functionalized surfaces and information storage. Azobenzene is a prototypical molecular switch owing to the trans-cis isomerization of the central double nitrogen bond. Low-temperature scanning tunneling microscopy and spectroscopy (STM/STS) are powerful tools for investigating molecular assembly and switching properties with high spatial resolution.

Here, we report a study on azobenzene tetramers which consist of four azobenzene moieties converging on a central tetrahedral carbon atom. After adsorption on Ag(111) surface, we find molecular aggregates with characteristic hexagonal shapes that can be assigned to periodic adsorption sites. The upright azobenzene unit of each species reversibly isomerize with constant time of few minutes either remotely by laser illumination or locally by the microscope tip. Moreover, our experimental

findings reveal that the molecular mobility depends on the isomeric state.

OGD-27 TALK 15:15-15:30 THURSDAY, SEP 13

HS BE01

Resonant excitation of helicene single molecules by radio-frequency scanning tunneling microscopy

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By supplementing our low-temperature (LT) scanning tunneling microscope (STM) with a custom radio frequency circuit we benefit, both, from high spatial resolution of STM and the exceptional energy resolution ($< \mu\text{eV}$) of magnetic resonance techniques. This setup allows the detection and excitation of mechanical [1,2], spin [3,4], and plasmonic [5] degrees of freedom on solid surfaces and adsorbates at cryogenic temperatures, maintaining sub-nanometer real-space resolution. In this presentation I introduce the distinctive features of our experimental rf-LT-STM system and report on resonant excitation of molecule-related eigenmodes of helicene derivatives adsorbed on Ag (111) in frequency range between 1 and 40 GHz.

[1] S. Müllegger *et al.*, *Phys. Rev. Lett.* **112**, 117201 (2014)

[2] S. Müllegger *et al.*, *Nanotechnology* **25**, 135705 (2014)

[3] S. Müllegger *et al.*, *Phys. Rev. Lett.* **113**, 133001 (2014)

[4] S. Müllegger *et al.*, *Phys. Rev B* **92** (2015) 220418(R)

[5] G. Serrano *et al.*, *Sci. Rep.* **7**, 9708 (2017)

OGD SESSION VI 16:00-17:30 THURSDAY, SEP 13

HS BE01

OGD-28 TALK 16:00-16:30 THURSDAY, SEP 13

HS BE01

Molecularly confined aqueous ionic liquid solutions

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Bio and aqueous applications of ionic liquids (IL) such as catalysis in micelles formed in IL solutions or extraction of chemicals from biologic materials rely on surface-active and self-assembly properties of ILs. Here we discuss qualitative relations of interfacial and bulk structuring of a water-soluble surface-active IL ([C₈MIm][Cl]) on chemically controlled surfaces over a wide range of water concentrations using both force probe and X-ray scattering experiments. Our data indicate that

IL structuring evolves from surfactant-like surface adsorption at low IL concentrations, to micellar bulk structure adsorption above the critical micelle concentration, to planar bilayer formation in ILs with <1 wt % of water and at high charging of the surface. Interfacial structuring is controlled by mesoscopic bulk structuring at high water concentrations. Surface chemistry and surface charges decisively steer interfacial ordering of ions if the water concentration is low and/or the surface charge is high. We also demonstrate that controlling the interfacial forces by using self-assembled monolayer chemistry allows tuning of interfacial structures. Both the ratio of the head group size to the hydrophobic tail volume as well as the surface charging trigger the bulk structure and offer a tool for predicting interfacial structures. Based on the applied techniques and analyses, a qualitative prediction of molecular layering of ILs in aqueous systems is possible.

OGD-29 TALK 16:30-16:45 THURSDAY, SEP 13

HS BE01

Tunable Swelling Behavior of Hydrogel Thin Films deposited by initiated Chemical Vapor Deposition

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Hydrogels are networks of hydrophilic polymer chains and water. Their ability to take up significant amounts of water (up to 10 times their dry size) makes them applicable in a variety of different frameworks (e.g., in drug delivery, contact lenses). Depending on the chemical composition, their characteristic water uptake behavior makes them particularly interesting for application in sensor and actuator setups. Diffusion as the time-limiting process in water ab- and desorption makes the use of thin films crucial to achieve fast response times. In this study, a series of thin hydrogel films are synthesized by initiated Chemical Vapor Deposition (iCVD) with varying deposition parameters such as film thickness (20-300 nm) or amount of crosslinking (0-50%). This solvent-free deposition technique allows for precise control over thickness and chemical composition. As a plethora of chemical compositions has been studied, stimuli-responsive (e.g., thermo-responsive) groups such as within N-Isopropylacrylamide (NIPAAm) have been applied to facilitate and investigate temperature-dependent swelling in terms of thin film properties. NIPAAm is the most prominent example of a hydrogel exhibiting a lower critical solution temperature (LCST), where it undergoes a phase transition between a “hydrophilic” swollen state below to a “hydrophobic” shrunken state above this temperature. The evolution of (polymer thin film) optical parameters are recorded by spectroscopic ellipsometry during swelling, as a function of temperature in humidity as well as fully immersed in water. These experiments allow for the detection of changes of the film thickness in the Ångström-range (e.g. thermal expansion) up to full swelling of the hydrogels with thickness increases of up to 150% of the dry film. An increasing amount of crosslinking has been found to lower the LCST, but also broaden the shape of the transition. On the other hand, lowering the film thickness lead to an increase of the LCST, whose magnitude depends on the crosslinker amount. These findings provide a promising basis for future sensing applications.

Finding new drug polymorphs within thin filmsM. Kaltenecker^{1,2}, B. Schrode^{1,2}, O. Werzer¹¹*Institute of Pharm. Sciences, Dep. for Pharm. Technology, University of Graz, Austria*²*Institute for Solid State Physics, Graz University of Technology, Graz, Austria*

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Defined drug crystallization is important as the therapeutic action strongly depend on the polymorph selection. Typically, the usage of bulk crystallization in solution is favored in pharmaceutical science as large amount of defined crystals can be processed. Often these methods are limited so that different preparation approaches are required for finding new polymorphs of higher benefit.

In this contribution we demonstrate how techniques typical used for thin film preparation can be used to access various polymorphic forms of model drugs. Employing grazing incidence X-ray diffraction and microscopy techniques the behavior of various systems could be studied in detail. Spin coating paracetamol enables film consisting of polymorphic form I, II or III. Further, the support of the solid substrate provides some stabilization for the form III which in general is metastable. The high temperature alpha and the room temperature beta form of caffeine results from variations in the solvent and film forming kinetics, i.e. how fast the solvent evaporates. Spin coating, drop casting and even vacuum deposition can be used to realize epitaxial growth of caffeine on single crystal surfaces. In a similar manner, experiments performed on nabumeton showed the capability to growth form I or II at surfaces dependent on the process kinetics. Furthermore, a new form was found which has been found just in proximity to a surface. Thus a labeling as a surface mediated phase may be justified. Another drug, phenytoin, was known to be monomorphic. Successful screening using thin film deposition techniques enabled finding a surface mediated polymorph. Employing grazing incidence X-ray diffraction, the structure was fully solved. From this knowledge we calculated that this new form has a lower lattice energy compared to already known polymorph. This contradicts other finding of simpler rod like molecules, for which a substrate mediated phase has in general a higher lattice energy. The higher dissolution rate of this new phenytoin phase explains by a change in the H-bonding network throughout the crystal.

In conclusion, the usage of thin film preparation techniques opens a variety of opportunities to find new polymorphs of potential high therapeutic profit. Further, the development of personalized medication requires also new fabrication routes to be established which are distinct from those typically applied in pharmaceutical industry. Hereby the thin film deposition methods might assist in achieving this goal in near future.

Crystallisation of dioctyloxy-benzthiophene within thin films: a layer-by-layer growth mode

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Thin films of the molecule benzthieno-benzthiophene (BTBT) are among the best materials of organic thin film transistors, since charge transport mobilities in the range of $10\text{cm}^2/\text{Vs}$ are observed. This study investigates the film forming properties of a specific BTBT derivative which is composed by octyloxy side chains at the terminal end of the conjugated molecular core. Thin films were prepared by physical vapour deposition on oxidized silicon wafers with defined surface energy. Starting from films with sub-monolayer thickness, to a single monolayer of up-right standing molecules proceeding up to multilayer films with a film thickness of 99 nm. The films are investigated by x-ray reflectivity (XRR) and grazing incidence x-ray diffraction to get thin film morphology and crystal structure. These integral characterization techniques were complemented by a microscopic technique using atomic force microscopy (AFM). In clear difference to commonly observed organic thin film growth scenarios, a layer-by-layer growth is observed. Grazing incidence X-ray diffraction reveals the formation of a thin film phase of the molecule which proves high crystallinity. The high uniformity of the film is proven by pronounced Laue fringes. Finally, the observed layer-by-layer growth mode is compared to other growth modes at the same substrate surface: pure island growth for the molecule dibromo-indigo and layer-and-island growth for the molecule pentacene.

Influence of thermal transport parameters on operation temperature of OLEDs

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Utilizing organic light emitting diodes (OLEDs) for lighting requires a homogeneous operation across large areas. OLED research mostly focuses on leveling electric properties, but also the thermal properties are expected to be highly relevant. Moreover, due to the peculiar coupling between thermal and charge transport in organics, these properties can not be decoupled from each other.

Therefore, it is crucial to understand how the temperature is distributed in the device and how temperature distribution in the organic layers affects the electric properties. For this task, thermal properties of the individual layers are highly relevant. Here we investigate the impact of two distinct heat transport parameters on the temperature distribution and current in OLEDs, namely (i) the thermal conductivity of the organic layers and (ii) the heat transfer coefficient between the device surface and the environment. We monitor the heat dissipation with a 3D drift-diffusion model that

self-consistently couples charge and heat transport.

We establish that the heat transfer coefficient is able to compensate unintentional device heating much more efficiently than the thermal conductivity of the organic layers. Intentionally elevated operating temperatures, that may improve the OLEDs electric performance, are not necessarily beneficial, as any increase in operating temperature decreases the device stability. We propose analytic expressions that aid the interpretation of the heat transport in terms of the two heat transport parameters.

PHYSICS-INDUSTRY

(PIN)

PIN SESSION I 14:00-15:20 WEDNESDAY, SEP 12

HS P3

PIN-1 TALK 14:00-14:20 WEDNESDAY, SEP 12

HS P3

Karriere als Physiker in der Industrie

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Die Ausbildung zum Physiker ermöglicht eine Vielzahl von Einsatzmöglichkeiten in der Industrie. Der Autor berichtet aus Erfahrungen seines Berufsweges, der ihn vom Ingenieur für Energiewirtschaft und Wärmetechnik bis zum Verantwortlichen für einen Unternehmensbereich von 160 Mio.EUR Umsatz mit 150 Mitarbeitern geführt hat.

Nach dem Studium der Technischen Physik und einer einjährigen Zusatzausbildung als Energieberater war die erste Berufsphase durch die Konzeption und Abwicklung von energie- und wärmetechnischer Projekte geprägt. Anhand von Beispielen werden die Erfolgsfaktoren von Projekten gezeigt, die zu wesentlichen Energieeinsparungen im Unternehmen geführt haben.

Mit der Übernahme der Führung der gesamten Energiewirtschaft am voestalpine-Standort in Linz sind die Aufgaben und die Verantwortung im technischen Management zunehmend angewachsen. Seit 18 Jahren ist der Autor am Standort Linz für den Bereich Strom zuständig. Das umfasst die Verantwortung für den Betrieb und das Asset Management des größten kalorischen Industriekraftwerkes Österreichs sowie des werksinternen Stromverteilnetzes, das eine Strommenge transportiert, wie sie die gesamte Stadt Linz benötigt.

Der Autor berichtet darüber, welche Fähigkeiten und Handlungsweisen für seine erfolgreiche Karriere nützlich waren.

PIN-2 TALK 14:20-14:40 WEDNESDAY, SEP 12

HS P3

Future Career Prospects for Physicists

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Holding a degree in physics is still a good foundation for a future career in multiple fields. Looking back in history, many successful physicists dedicated their life to science. For the best ones, this effort was awarded with a Nobel Prize, which made their groundbreaking work transparent to the public as well. In the last two decades, however, driven by the need of new technology and products, a variety of new degree programs occurred. Even though the knowledge and skill set of physicists makes graduates attractive to the industry, additional competences are required. This leads to the

following questions:

1. Which competences make physicist outstanding and which additional skills are important?
2. Which industries are currently looking for physicists?
3. Who are the role models and global influencers?

A good example is Elon Musk, the founder of Tesla and Space X. He is one of the biggest global influencers in the industries of e-mobility and renewable energies. As a physicist, he has distinct analytical skills, a high competence in problem solving and he can create visionary ideas. In addition to his scientific background, he has build up know-how in various fields of technology (space and car engineering, renewable energies), software development and entrepreneurship.

In todays' working environment, life-long learning is crucial for everyone. Due to their education physicists have high competencies that qualify them for multiple jobs. Besides of a career in science, this can be as software developers, data scientists, managers, entrepreneurs, or inspiring leaders. However, at the end we should have in mind that being a physicist is not a profession. It is a passion. A passion that opens new career paths and opportunities in politics, society and industry.

PIN-3 TALK 14:40-15:00 WEDNESDAY, SEP 12

HS P3

Physics as foundation for innovations in industry

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Innovation, the three-stage process is well described by Josef Schumpeter, as one of the basic principle of economics, but there is no guideline on how are they generated. The demand on innovations in/for the industry is raising, even more never ending. One of the most reliable sources, which is able to generate a continuous flow on innovations, is physics.

This talk will show perspectives of innovations in general and how integrated physics are driving the innovation-motor of an industry. Within ten years, physics as method have transformed a small metalworking-company into an international technology group with inhouse research, international investors and latest products for e.g. smart cities.

In addition to methodological findings, examples are presented to illustrate the results of the integration of physics into industry. First and foremost is the Science Tower Graz: ambassador and pioneer for a sustainable future based on methods of physics!

PIN-4 TALK 15:00-15:20 WEDNESDAY, SEP 12

HS P3

Study, Research, Teaching and Management, over a period of 35 years

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After having finished the Matura at the BRG Villach 1980 the author started with the study of technical physics at the TU Vienna in 1981. There, in higher semesters the author also engaged in teaching as a tutor in computing exercises and compulsory laboratories. In addition to the experimental investigation of a mixed crystal series $(Ce(Al_{1-x}T_x)_2)$, $T = Cu$ or Ni , the main focus of the diploma thesis was laid on the automation of several measuring systems, which until then had been operated

by hand. After spending several months abroad at the CNRS in Grenoble, France, the doctoral program began in 1990, where several new measuring methods were set up, as well as a variety of highly-correlated electron systems were studied. From this, a large number of publications were derived, of which about 25 formed the core of the dissertation, which was completed in 1996 after a longer stay abroad in Kumamoto, Japan. The subsequent post-doctoral phase lasted until about 2000 and was marked by further research stays in France and England, further publications and lectures at conferences and workshops as well as continuing teaching at the TU Vienna.

At about 2001, the author switched to a non-university research center (CTR in Villach), where he initially worked as a key researcher, later as a group leader, in industry-related projects, with e.g. AVL or EGO. He built both a new branch of research and a new business field employing SAW sensor technology.

Around 2006, the change to the FH Kärnten took place, where the author has since held the professorship for technical physics. In 2013, he took over the newly established mechanical engineering degree course, for which he is still responsible. Since the beginning of 2017, the author also acts as spokesman of the Energy Working Group of the ÖPG.

Poster Contributions of Divisions

ATOMS, MOLECULES, QUANTUM OPTICS and PLASMAS

(AMP)

AMP-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

A comparison of machine learning algorithms for transition state searches in computational chemistry

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Accurate reaction pathways are essential for realistic predictions of chemical reactivity as well as for correct estimates of product distributions. Well established methods such as the nudged elastic band approach, the growing or freezing string method or eigenvector following techniques are typically applied to molecular systems. However, all these approaches have in common that a sufficiently large set of data points is required. Often, large basis sets and expensive post-Hartree-Fock methods or advanced density functionals need to be applied, which makes the necessary pointwise evaluations very time consuming, especially in the case of larger systems with complicated, high-dimensional potential energy surfaces (PES).

Reaction pathway searches can be accelerated by machine learning techniques. Two promising approaches, namely the neural network and Gaussian process regression, have been proposed. In our study, we compare these two machine learning strategies with ridged regression and support vector machine implementations. A big advantage of all four algorithms in comparison to standard evaluations of the reaction pathway is the additional information gained about the local shape of the PES. Here, Gaussian process regression is particularly interesting as it automatically provides an error estimate for the prediction.

The four methods mentioned above are tested on well-known benchmark systems with respect to the minimum energy path accuracy, computational expense and their predictive power. The last point, the ability to predict PES curvature, focuses on local regions near the reaction pathway, i.e. parts of the PES which are highly relevant for dynamical studies of branched reactions.

AMP-2 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Applicability of Neural Network-based Approaches to SCF Initial Guess Generation

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Self-consistent field (SCF) iteration algorithms of Hartree-Fock implementations in computational chemistry have seen numerous improvements in the last decades. Yet, many of the initial guess generation methods currently in use still suffer from systematic deficiencies. Convergence for e.g.

large metallic systems is still problematic in many cases and 'black box'-type initial guesses often apply only to a limited selection of standard basis sets. An inappropriate guess can lead to a very slow and therefore inefficient convergence behavior. In spite of the large efforts that have been made in order to develop more sophisticated and generic variations of standard methods (e.g. superposition of atomic densities or Hückel-based methods), most of the more advanced schemes can be applied effectively only in a narrow range of scenarios.

Hückel-based methods are very effective for organic molecules. Metallic systems, on the other side, are preferably treated via the conceptually simple superposition of atomic densities. However, this approach does not provide molecular orbitals directly, and basis set projections are often limited to an implemented subset of standard basis functions. These shortcomings motivate the quest for a more general ansatz, e.g. based on machine learning algorithms. We shed light on the applicability of a neural network-based approach in order to find fast converging initial guesses for the SCF algorithm. In our current study, molecular geometry and chosen basis set are the only inputs fed to the network.

AMP-3 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Subradiance in V-type Multi Level Systems

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Spontaneous emission in quantum emitters can be modified by other emitters nearby, leading to super- and subradiance. We demonstrate the subradiant behaviour of V-type multilevel emitters in close vicinity to each other, with specific examples being an equilateral triangle and a linear chain at interatomic distances below the transition wavelength. For the equilateral triangle an analytical treatment is possible for a very symmetric configuration. In this setup the Hamiltonian features a maximally entangled, antisymmetric eigenstate involving superpositions of all three atoms which exhibits subradiance as opposed to superradiance. Moreover, it decouples completely from the vacuum radiation field and therefore does not decay spontaneously. Numerical simulations involving different dipole orientations and interatomic distances are presented and their subradiant properties are investigated as well.

AMP-4 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Majorana bound states in monoatomic Fe-nanowires on superconducting Pb

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Motivated by their potential use as topological qubits, Majorana bound states (MBS) have attracted an utmost interest. Theoretical calculations predict their occurrence in the combination of quasi-one-dimensional nanowire systems onto s-wave superconductors.

Here, we measure the spatial and electronic characteristics of topological, superconducting chains of iron atoms on Pb(110) to investigate the wave function and the localization length as finger-

print for MBSs [1]. After first observations by scanning tunneling microscopy (STM) [2,3], we demonstrate by combining STM and atomic force microscopy (AFM) at low temperature (< 5 K) that the Fe chains are mono-atomic, structured in a linear fashion, and exhibit zero-bias conductance peaks at their ends [4]. This can be interpreted as signature for a Majorana bound state [5].

From these observations, we strongly support the idea of using MBSs in Fe chains on superconducting Pb as qubits for quantum computing devices.

- [1] Klinovaja J. & Loss, D.; *Phys. Rev. B* **86**, 085408 (2012)
- [2] Nadj-Perge, S. *et al.*; *Science* **346**, 602 (2014)
- [3] Ruby, M. *et al.*; *Phys. Rev. Lett.* **115**, 197-204 (2015)
- [4] Pawlak, R. *et al.*; *npj Quantum Information*, 16035 (2016)
- [5] Mourik, V. *et al.*; *Science* **336**, 1003 (2012)

AMP-5 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Photofragmentation of Corannulene cations solvated in helium droplets

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The special properties of superfluid helium nano droplets (HND) [1] can be used to reproduce the harsh conditions of the interstellar medium (ISM), which makes this cryogenic matrix a perfect laboratory for the investigation of potential carriers of a diffuse interstellar band (DIB). Possible candidates are carbon containing complexes like the polycyclic aromatic hydrocarbons (PAH).

The HND via supersonic expansion and doped by individual pick-up with Corannulene molecules. Inside the HND $(C_{20}H_{10})He_n$ complexes are formed and are cooled to ultra-cold temperatures. Subsequently the clusters are ionized via electron bombardment and analyzed by a commercial high resolution time-of-flight mass spectrometer (TOF-MS) where spectra were recorded with respect to the m/q ratio [2].

In addition the ions can be excited by a tunable laser beam (EKSPLA NT240-SH-K1), which is synchronized with a given extraction pulse of TOF-MS. The depletion of the measured ion yield of the irradiated complexes shows absorption lines, The resonances show a remarkable redshift up to 32 helium atoms for the $(C_{20}H_{10})^+He_n$ complexes.

This work was supported by the FWF (Project numbers P26635, P31149 and W1259), and the European Commission (ELEVATE, Horizon 2020 research and innovation program under grant agreement No. 692335)

[1] Toennies, J.P. and A.F. Vilesov, Superfluid helium droplets: A uniquely cold nanomatrix for molecules and molecular complexes. *Angewandte Chemie-International Edition*, 2004.**43**(20):p.2622-2648.

[2] Schöbel, H., Bartl, P., Leidlmair, C., Denifl, S., Echt, O., Märk, T. D. and Scheier, P., High-resolution mass spectrometric study of pure helium droplets, and droplets doped with krypton. *The European Physical Journal D-Atomic, Molecular, Optical and Plasma Physics*, 2011. **63**(2):p.209-214.

A superradiant clock laser on an optical lattice with moving atoms

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It is theoretically well described that an ideal superradiant laser on an optical clock transition with fixed positions of the atoms features an extreme frequency stability and accuracy. To obtain a more realistic description we extend this model by adding classical positions and momenta of the atoms to the system as dynamic variables. We study the properties of the spectrum of such a laser as well as its stability. For well chosen parameters we predict a stable atom configuration inside the cavity. Further, the atoms are simultaneously cooled via stimulated cavity cooling and thus the trapping in the cavity direction is achieved by the system itself. The dynamics of the atoms does not depend that much on their initial positions and momenta as soon as they are initially cold enough. We find that the shape of the laser spectrum is only weakly shifted when compared to the case of atoms at fixed positions.

Size Distributions of Helium Nano Droplets

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Super fluid helium droplets are frequently used in experiments as a super cold matrix for the analysis of molecules and atoms. In recent experiments, size distributions of helium nano droplets formed in free jet expansion¹ have been analyzed. Since the cross section in the pickup process directly corresponds to the size of the droplet, a good knowledge of the size distributions in the beam is crucial. In experiments like those entailing the formation of superfluid helium nano droplets doped with clusters of C₆₀ and smaller molecules², the super cold matrix of the helium droplets is used. Furthermore, the size of a droplet affects how much energy can be dissipated from its dopants due to evaporative cooling.

The helium droplets are formed in a free jet expansion with a nozzle diameter of 5 μm at temperatures of 4 K to 9 K. The droplets are then ionized via electron impact ionization with low electron energy in order not to alter the size distribution. Using an electrostatic analyzer, the droplets are filtered according to their mass to charge ratio. A channel electron multiplier is used to detect the charged particles. However, this method is limited by the maximum electric field that can be applied to the deflector plates and the dimensions of the analyzer. For the present setup the largest singly charged droplet that can be deflected contains about 35 million helium atoms.

In another approach, the helium droplets are ionized more strongly in order to create multiple charges in the droplets. These multiply charged helium droplets provide a method the study the size distribution of much larger droplets.

[1] L. F. Gomez et al., Sizes of large He droplets, *The J. of Chemical Physics* **135** (2011)

[2] Schöbel, H. 2012. Electron ionization of superfluid helium nanodroplets doped with C₆₀ and small molecules. *J. of Physics: Conference Series* 388: 012044.

Multiply charging of superfluid helium nano droplets

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Superfluid helium nano droplets have been widely used as a cryogenic matrix in studies of complexes such as gold clusters¹. To provide better insight on the nature of superfluid helium nano droplets and their interaction with embedded dopants, the influence of electron impact ionization on pristine superfluid helium nano droplets has been investigated. Positively charged droplets with uniform velocity, produced via supersonic jet expansion and electron impact ionization, are mass selected in an electrostatic sector according to their kinetic energy. The charged droplets are then again subjected to electron bombardment and separated for their mass to charge ratio by a second electrostatic sector. Multiply charging of selected droplets can be observed. Depending on ionization parameters and droplet size the resulting mass to charge distribution of the product droplets varies greatly. These findings spur the development of a mechanism for producing multiple size selected dopant clusters in a single helium nano droplet.

[1] M. Goulart *et al.*, *Phys. Chem. Chem. Phys.* **14**, 9554-9560 (2018)

CONDENSED MATTER**(COND)****Thermal transport in metal-organic frameworks from first principle calculations**

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Metal-organic frameworks (MOFs) have been intensively studied during the last years due to their numerous possible applications, for example in gas absorption and catalysis. In spite of their importance, the heat transport properties of MOFs are rarely investigated, although they are crucial for many applications (e.g. heat dissipation, thermoelectricity). The presence of very heavy and light atoms in the unit cell can lead to low-frequency optical phonon modes that typically have a high contribution to the thermal conductivity, which complicates the situation.

Moreover, the ability to change the constituents of MOFs opens the possibility to design materials with tailor-made thermal transport properties: by using anisotropic linker structures also preferred pathways for thermal transport can potentially be realised. This calls for gaining an in-depth understanding of the heat transport in MOFs. To achieve this, we present a study dealing with the influences of different constituents on the thermal conductivity to deduce reliable structure-to-property relationships. Starting from MOF-5 a systematic variation of (i) the metal nodes (Zn, Mg, Ca) and (ii) the organic linkers (different aromatic molecules, functional substituents, alkynes) is performed.

Atomistic simulations are carried out in the framework of density functional theory (DFT) and density functional tight binding (DFTB). The thermal conductivity tensors for various MOFs are calculated using the model proposed by Bjerg et al.¹ relying on the Boltzmann transport equation (BTE) within quasiharmonic lattice dynamics.

[1] Lasse Bjerg, Bo B. Iversen, and Georg K. H. Madsen. Modeling the thermal conductivities of the zinc antimonides $ZnSb$ and Zn_4Sb_3 . *Phys. Rev. B*, 89:024304, Jan 2014.

COND-2 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Structure-to-property relationships for heat transport in organic semiconductors

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The low intrinsic thermal conductivity of organic semiconductors is a limitation for applications in which heat is dissipated and has to be transported away from the active region. Conversely, it is a huge advantage for thermal barriers or thermoelectric usage. Even for non-thermal related applications it is important to know about mechanisms that govern the transport of heat. Despite its importance, the area of thermal transport in organic semiconductors is almost uncharted. The present work aims for a better understanding of heat transport in crystalline organic semiconductors by revealing the corresponding structure-to-property relationships. To that aim, density-functional-tight-binding (DFTB) calculations are employed to study the phonon structure of a series of carefully chosen test systems. The thermal conductivity tensor is obtained by using a quasiharmonic lattice dynamics approach as proposed by Bjerg et al.¹ that uses the mode Grüneisen parameter. Our results illustrate, how the thermal conductivity of an organic semiconductor is impacted by the material's chemical structure varying the chain length of the molecules, comparing flexible (biphenyl) and rigid (fluorene) structures, and highlighting the impact of anisotropy in a prototypical conjugated polymer (poly-1,4-phenylene).

[1] Bjerg *et al.*, *Phys. Rev. B* **89**, 024304

COND-3 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

The interplay of Ion Transport and Polarizability in Li_6PS_5X (X: Cl, Br, I) as probed by Impedance and Raman Spectroscopy

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The realization of solid-state-lithium-based batteries needs suitable solid electrolytes. Over the last couple of years, design strategies and structure principles, as well as attempts at generalization have been presented to explain the origins of 'superionic' conduction in solids.

Since several years lithium argyrodites with the general formula Li_6PS_5X (X: Cl, Br, I) have been introduced as promising electrolytes. Although several studies already reported on ionic conductivi-

ties and on test cells using argyrodites as solid electrolytes, a clearer picture of the relevant factors that promote its superionic behaviour is needed. Ionic conductivity is governed by (i) the effective number of charge carriers and (ii) their mobility. Compounds with extensive lattice disorder and many unoccupied regular or interstitial sites often show rapid cation movements, as far as these sites are connected by low energy pathways. Other factors are (iii) the size of the mobile ions, (iv) the ionic charge, (v) the (local) bonding character, *i.e.*, the preferred coordination of the ions and whether ionic, covalent or mixed bonding is present, and (vi) the polarizability of the immobile ions. The latter, together with the crystal structure, directly affects the potential landscape the mobile ions are exposed to. Partial replacement of the sulfur anions in $\text{Li}_6\text{PS}_5\text{X}$ with distinctly polarizable anions, such as Cl, Br, and I, is expected to influence local ion jump processes and macroscopic ion transport.

In our study we used broadband conductivity spectroscopy, carried out over a large frequency range, to study conductivities, activation energies and prefactors of the underlying Arrhenius behavior in combination with Raman spectroscopy to study the polarizability of the crystal lattice. Preliminary results on the interplay of ionic transport and the polarizability will be presented.

COND-4 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Characterization of Tannin-Furanic Foams by Raman Spectroscopy, Infrared Spectroscopy, and by X-ray Computed Microtomography

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The main goal of this research activity is the characterization of totally natural rigid foams, derived from byproducts of wood industries (such as tannin and lignin) at the nano, micro and macro level through the exploitation of state-of-the-art spectroscopic techniques combined with imaging and mapping options, employing a wide range of electromagnetic radiation from far infrared to X-rays.

The tannin-based foam formation is an acid-catalysed polymerization involving a self-blowing reaction in which the foam raises up introducing a preferential direction of growing. This foam synthesis is a crucial point influencing internal chemical and morphological variations which might affect the macroscopic properties of the foam as final product, since the correlation between structure and degree of pore connection, as well as the chemical nature of the skeleton and surfaces of the walls, play a fundamental role for steering the most appropriate applications. The synergistic complementation of several analytic techniques (Raman spectroscopy, infrared spectroscopy, X-ray microcomputed tomography), available as a cross-border infrastructure via a cooperation between Elettra Sincrotrone Trieste, University of Salzburg and Salzburg University of Applied Sciences within the Interreg Italy-Austria ITAT1023 InCIMA project (2017-2019), will enable to optimize, in future subsequent steps, these materials with potential applications as new materials for green-building technology (e.g. thermal and acoustic isolation) and for natural filtering systems (e.g. water purification from contaminants of emerging concern).

We acknowledge financial support provided by Central European Research Infrastructure Consortium through the proposals CERIC 20167027 and 20177080.

We acknowledge financial support provided by the European Regional Development Fund and Interreg V-A Italy-Austria 2014-2020 through the Interreg Italy-Austria project ITAT 1023 InCIMA

COND-5 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Interplay of intermolecular electronic coupling and crystal structure in quinacridone

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Organic semiconductor crystals are materials that combine semiconducting properties with the chemical and mechanical benefits of organic materials. They are typically held together by comparably weak van der Waals interactions, which results in a wide variety of structures with similar energies referred to as polymorphs. These different polymorphs (crystalline packing states) can have very different electronic properties, either qualifying or disqualifying them for certain electronic applications. Thus, it is important to investigate and understand the interplay between crystal packing and intermolecular electronic coupling. We investigate this interplay by employing dispersion-corrected density-functional theory to calculate the electronic structure of the three stable and structurally very different polymorphs of quinacridone. It is found that within the α -polymorph, being almost perfectly π -stacked, the direction of the intermolecular H-bonds is the one with the largest intermolecular electronic coupling, at variance with our initial expectation that transport along the $\pi - \pi$ stacking direction should dominate. To understand that, we study the strength of the intermolecular electronic coupling, the resulting band-widths, as well as the relevant effective masses, as a function of the shift of the molecules along the long molecular axis. It is observed that, for an artificially built coplanar quinacridone crystal, the intermolecular electronic coupling oscillates as a function of the displacement along the long molecular axis consistent with what has been previously observed in dimer calculations, e.g., by Coropceanu et al.¹ Notably, the evolution of the coupling is in line with that of the total energy, suggesting that there is a natural driving force in organic semiconductors to minimize the (non-bonding) electronic coupling rendering high-mobility structures energetically unstable upon self-assembly.

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COND-6 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Correlative Scanning Electron Microscopy and Raman Microscopy – Synergies and best Practices

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With RISE (Raman Imaging and Scanning Electron Microscopy) a new method has recently been established at the FELMI-ZFE Graz. This new method combines two microscopic techniques, namely

high resolution scanning electron microscopy (Sigma 300 VP; Zeiss, Germany) and chemical imaging using Raman microscopy (RISE; WITec, Germany). Additionally elemental analysis using energy dispersive X-ray spectroscopy (EDXS) is possible. This unique combination of three techniques offers new possibilities for the microscopic analysis of a wide range of samples, as Raman microscopy can provide information about chemical bonds (especially H-bonds) as well as organic components that would usually not be available using the combination of SEM and EDXS. Even on anorganic samples Raman spectroscopy can provide complementary information about oxidation states and crystal structure. Here we provide some examples from specific samples that demonstrate possible synergies between Raman and scanning electron microscopy. These examples include a larger variety of materials such as polymers, metal oxides, metal-organic compounds, geological samples, pharmaceuticals and building materials. Additionally we give insight into the necessary sample preparation steps for correlative Raman-SEM microscopy, as well as point out some of the practical pitfalls and limitations one might encounter.

COND-7 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Accessing the Internal Morphology of Nano-Granular FEBID Materials in 3D Space by Electron Tomography

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Focused electron beam induced deposition (FEBID) is an additive, direct-write fabrication technique that enables controlled material deposition of nanoscale structures on virtually any given surface. Typically, organometallic precursors are used, e.g. MeCpPtMe₃, resulting in nano-granular materials composed of metallic nano-grains (e.g. Pt) spatially embedded in carbonaceous matrix [1].

The distances between individual grains as well as the chemistry of the carbon matrix significantly influence electrical [2] and mechanical [3] functionalities, which form the basis for potential applications of FEBID structures, such as gas sensing via nanoscale resonators or functionalized tips for advanced atomic force microscopy (AFM). To understand the relation between morphology and properties, conventional two-dimensional (2D) projection images are insufficient, thus three-dimensional (3D) structural analyses are indispensable. For this purpose, electron tomography is an appropriate technique, where 3D morphological information can be reconstructed from a tilt series of 2D projections.

In this first approach, we investigate nanogranular Pt-C FEBID deposits before and after post-growth e-beam curing, as recently applied for tuning the Young modulus in resonant sensor applications. By using scanning transmission electron microscopy (STEM) tomography, we reconstruct free-standing FEBID deposits in 3D space, which yields sizes, shapes and spatial distribution of Pt grains together with their intergrain distances. Based on the results, we study the implications of post-growth e-beam curing on internal grain sizes, shapes and their spatial distribution. We attempt to link this information to measured mechanical properties of FEBID materials before and after e-beam curing.

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COND-8 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Oxide Ceramic-Electrode Systems: STEM EDXS Analyses and Heating Experiments

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Oxide ceramics are widely used in a variety of engineering applications in microelectronics. Electric properties of electronic devices depend on design, used material systems, doping, and process control. Dopants may on the one hand blend in the crystal lattices or on the other hand accumulate in grain boundaries or at the interface between material and electrodes. Furthermore, the electrode material may diffuse into the ceramic during production processes.

Analysing the micro- and nanostructure remains a cornerstone, when it comes to high-end manufacturing in this field. We use scanning transmission electron microscopy (STEM) and energy-dispersive X-ray spectroscopy (EDXS) to examine the material at the nanoscale. With respect to quantitative analysis, oxide ceramics, as in our case lanthanum-doped lead zirconate titanate (PLZT), are a complex and challenging task. Absorption effects occur in the material, which influence quantification results. Additionally, the sample preparation of very thin TEM lamellas is demanding, since PLZT bends heavily when being thinned.

We worked with PLZT multilayers deposited between copper electrodes and investigated diffusion processes, dopant behaviour and perturbing effects in stoichiometry. Our analyses reveal an increase of Cu in the material towards the electrodes, which indicates diffusion during manufacturing. Moreover, we found an enrichment of zirconium oxide grains at the interface between the electrode and the ceramic. Furthermore, we detected several single PLZT grains with inhomogeneous composition: an increase of lead and a reduction of titanium and lanthanum in grain centres. Finally yet importantly, we examined thermally driven changes of the material. *In situ* heating experiments revealed a severe change in the ceramic material at 700°C where strong elemental shifts appeared: areas of zirconium oxide formed.

Our subsequent work will focus on the material behaviour at the atomic scale, e.g. dopant position in the crystal lattice. Therefore, we have already started to perform High-Resolution-STEM measurements in combination with EDX spectrum imaging.

The authors thank EPCOS OHG, A TDK Group Company for the samples and the Austrian Research Promotion Agency FFG (project 850220/859238) for funding.

COND-9 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Mode shifting due to spin polarization in single layer graphene on a substrate

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Graphene, an almost purely two dimensional system, has opened up new doors into modern electronics. The growing precision of optical and scattering experiments necessitates a better understanding of the influence of damping on the collective mode of electrons or holes in such sheets. Further, the spin of the charge carriers is a promising candidate as an independently manipulable information carrier in electronic devices, heading towards spintronics.

We report spin-sensitive partial and full linear response functions of graphene, which give access to charge- and spin-density related excitations. In contrast to two dimensional electron liquids in heterostructures, graphene's collective mode can be strongly Landau-damped even at small wave vectors, due to single-particle interband transitions. Increasing the spin-imbalance of the free charge carriers in Dirac materials significantly broadens and shifts the plasmon. This enables to switch its lifetime (its mean free path) by tuning the spin polarization of graphene, thus, in turn, to switch the efficiency of appliances coupled to this mode.

To bring our results to the test, we calculated the reflectivity of graphene on a SiO₂ surface, as observed in s-wave scanning near field microscopy. The above shift in mode position affects the dipole interaction function, a key quantity of the measurement. We also predict an antiresonance in the longitudinal magnetic response, similar to that in semiconductor heterostructures.

NUCLEAR and PARTICLE PHYSICS

(FAKT)

FAKT-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

***q*BOUNCE: current status of the Ramsey-type GRS experiment**

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In the past years, the *q*BOUNCE collaboration designed and built a new Ramsey-type experiment for gravitational resonance spectroscopy (GRS) with ultracold neutrons (UCN) in order to increase the sensitivity for tests of Newton's gravitational Law at small distances. Since the end of 2016, the setup is situated at the Institute Laue-Langevin (Grenoble). Presently, we are finalizing the planned measurements during another 100 days of beam time in France.

We will present the status of the measurements and give an outlook of future extensions of the Ramsey-type setup.

Search for Neutron Decay into Dark Matter Particles

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The neutron life-time plays an important role, both in cosmology and particle physics. Beam and storage experiments yield results with a significant deviation. A recent publication shows the possibility to explain this effect by proposing a decay of the neutron into a dark matter particle. One of the proposed decay channels is $n \rightarrow \chi + e+e-$, where χ is a dark matter particle with a mass similar to mass of the neutron. We are currently re-analysing data taken by the PERKEO II experiment at the ILL, dedicated to determination of the electron asymmetry parameter A . Since the experiment is sensitive to the proposed decay mode, we explore the possibility to set limit for this branching fraction. With this poster we will present the status of the analysis.

The CLIC detector

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The Compact Linear Collider (CLIC) is a future electron-positron collider currently under study. It foresees electron-positron collisions at centre-of-mass energies ranging from a few hundred GeV up to 3 TeV. CLIC offers a rich precision physics program, and a high sensitivity to a wide range of possible new phenomena. The precision required for such measurements and the specific conditions imposed by the CLIC beam structure put strict requirements on the detector design and technology developments. This includes ultra-low mass vertexing and tracking systems with small cells, highly granular imaging calorimeters, and a precise hit-timing resolution for all subsystems. Ambitious R&D programs for silicon tracking detectors and calorimeters are pursued, addressing the challenging detector requirements with innovative new technologies. A variety of detector optimisation studies have been carried out to establish the overall detector performance and to assess the impact of different technology options. The resulting optimised detector model has been integrated in the CLIC full-detector simulation framework. This contribution reviews the optimisation studies performed for critical parameters of the CLIC detector, presents the detector performance achieved in full-detector simulations, and gives an overview of the ongoing hardware R&D.

Simulation and optimization of a setup for proton computed tomography at MedAustronE. Ulrich-Pur¹, A. Burker¹, A. De Franco², L. Sihver^{1,2}, T. Bergauer³, A. Hirtl¹¹*Atominstytut, TU Wien, Vienna, Austria*²*MedAustron, Wiener Neustadt, Austria*³*Institute of High Energy Physics, Vienna, Austria*

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Proton therapy uses accelerator-produced proton beams to treat deep-seated tumours. The main advantage of proton therapy is the sparing of normal tissue during treatment due to the depth-dose characteristics of the proton beam, exhibiting the so-called Bragg-peak close to the end of the proton range.

In addition to accurate verification procedures, assuring the proper patient position during treatment, proton therapy requires valid predictions of the proton range and dose deposition. One method to achieve this goal is proton computed tomography (pCT), which measures the energy loss of protons at the plateau of the Bragg curve.

At the moment, MedAustron uses 62.-252.73 MeV protons for therapy and will be able to use protons up to 800 MeV by the end of 2019. Such high proton energies are not useful for therapy but essential for imaging and are rarely available in other centers designed for proton therapy, of which the vast majority is based on small sized cyclotrons.

The detectors used for pCT, however, require lower particle rates ($10^5 - 10^6 \text{ s}^{-1}$) than those currently used for patient treatment at MedAustron ($\sim 10^{10} \text{ s}^{-1}$). Therefore different particle flux reduction methods had to be established and tested experimentally at MedAustron. For this purpose a beam monitor, consisting of plastic scintillators and a FPGA based VME logic was developed and optimized. Particle fluxes down to 10^4 s^{-1} could be measured and are now available at MedAustron.

In order to calculate the particle range in the patient correctly, the path of the traversing proton has to be estimated. Therefore, a tracking telescope, consisting of four double-sided silicon strip detectors was set up then simulated with Geant4 and tested experimentally. The scattering power of a plastic phantom, mounted on a rotary table, was measured and compared to the Geant4 simulation. Additionally, several parameters influencing pCT were investigated. The results of the experiments and the simulations are presented.

MEDICAL PHYSICS, BIOPHYSICS and ENVIRONMENTAL PHYSICS

(MBU)

MBU-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Structural Characterization of 3D printed Samples - using Fused Deposition Modeling - consisting of different Biogenic Wood Filaments

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Fused Deposition Modeling (FDM) has become a very common and widespread Additive Manufacturing (AM) technology, being successfully exploited in a wide range of completely different industries for manufacturing thermoplastic parts. While processing, a thermoplastic material - designated as filament - is melted in the hot end, forced through a nozzle and finally deposited layer by layer until the 3D component is completed. A wide range of applicable materials, very low costs for production, as well as minimum material waste, are some of the benefits of Additive Manufacturing, especially FDM.

The biogenic wood filaments used for producing the three-dimensional test specimens are a composite material consisting of thermoplastic Polylactic Acid (PLA) and a varying proportion of wood fibers as well as wood particles, the proportion depending on the filament producer.

One task of this research work is the Raman spectroscopic characterization, i.e. the determination of the filament's composition with respect to chemical compounds, of several 3D printed test samples, each consisting of a different biogenic wood filament, partly from various manufactures. The Raman spectra of the examined test specimens were compared with the spectrum of pure PLA as reference, in order to be able to detect any possible compositional and structural variance within the samples. In addition to the assignment of all detected Raman peaks, chemometric techniques - i.e. multivariate statistical analysis methods including cluster analysis as well as factor analysis - were carried out enabling to classify and differentiate the Raman spectra of the specimens with respect to the reference spectrum of pure PLA.

This research activity is implemented within the Interreg Austria - Bayern AB 97 TFP-HyMat project. The major aim of this cooperation is the establishment of hybrid materials, in our case utilizing biogenic 3D printing wood filaments for FDM.

RESEARCH with NEUTRON and SYNCHROTRON RADIATION

(NESY)

NESY-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

SASHEL: Dummy Atom Modelling of Elongated Nanostructures from Solution Scattering Data

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Small angle scattering (SAS) is an established technique to study structural aspects, such as size and shape, of molecular systems in solution. As this structural information is not directly apparent from the recorded scattering intensity, one requires a fitting process that relies on an underlying mathematical model often limited to a specific shape [1]. Dummy atom (DA) modelling, so describing the particle shape as a variable bead assembly, bypasses this issue as the fitting process is not anymore constrained to a single geometry [2]. While current DA modelling implementations [2,3], which are predominantly based on the spherical harmonics approximation, have nourished several outstanding scientific advances, they show difficulties when applied to highly asymmetric particles, such as helical- or fiber-like structures [4].

We present a bead-modelling algorithm to determine the structural motif of monodisperse, highly-elongated systems in solution from SAS data [4]. We use symmetrical boundary conditions to project the seemingly infinite nature of e.g. helical systems onto a single building-block unit, represented by dummy atoms (DA). Departing from current practices, the building-block is altered by random DA movements while simultaneously fitting the corresponding scattering curve against the experimental one. Throughout the fitting process, an antifragile contribution is critical that repeatedly forces (un)favorable random movements onto each DA. Model and experimental scattering patterns are used to evidence functionality of the fitting algorithm. Its implementation is the program SasHel (available at <http://sashel.tugraz.at>).

NESY-2 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

***In situ* SAXS/XAS characterization of Proton Exchange Membrane Fuel Cell - a preliminary study**

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The high cost of platinum, used as a catalyst in Proton Exchange Membrane Fuel Cells (PEMFCs) led

the research to substitute it with Pt alloys whose coarsening and degradation at the electrodes is one of the main causes of reduced stability and premature aging for PEMFCs. A complete understanding of Oxygen Reduction Reaction and Hydrogen Evolution Reduction at the electrodes could lead to future improvements in fuel cell design. To investigate the catalytic activity on both chemical and structural level in situ SAXS and XAS spectroscopy would allow both short range and overall structure investigation. The results from both techniques, at different electrochemical conditions as well as during accelerated stress tests, would provide insights into chemical and structural degrading effects such as Pt coalescence and dissolution of the CeO₂ or Co matrix, respectively. Results from preliminary studies, which further let do *in situ* characterization of the complete fuel cell, are shown.

SURFACES, INTERFACES and THIN LAYERS

(OGD)

OGD-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Epitaxial growth of the acene and phenylene based fiber-like crystallites on large-area MoS₂ mono-layers

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Our study addresses the epitaxial growth of organic one-dimensional (1D) fiber-like nanostructures on the two-dimensional (2D) semiconducting substrate molybdenum disulfide. Due to the van der Waals nature of the interface between the semiconductor molecules and the substrate, the fibers are rotationally commensurate regardless of the lattice mismatch. These nanostructures form through self-assembly and self-alignment highly ordered networks of p-n junctions with the 2D substrates. The resulting mixed-dimensional (1D-2D) heterostructures could therefore be used in many optoelectronic and sensing applications due to their high light-matter interaction, possibility for photo-excited charge separation, and strong dependence of these interactions to light polarization.

Chemical vapor deposited (CVD) films of mono-layer MoS₂ - with over 100 μm wide single-crystalline grains - are used as a substrate [1-3] for the epitaxial growth of organic semiconductor nano-fibers. Two different types of small rod-like molecules are grown by hot wall epitaxy method. The resulting growth morphologies are investigated by atomic force microscopy. The molecules are chosen in such way that their backbones (acene or phenylene) resemble the packing motif of MoS₂ in either armchair or zigzag directions. As a consequence of this structural resemblance, the site specific adsorption of the two different molecular species follows the different high-symmetry directions of MoS₂. Our preliminary results indicate that in the case of parahexaphenyl (phenylene backbone) the molecules adsorb with their long axis along an armchair direction of MoS₂ with the resulting fiber-like crystallites growing in zigzag directions. In the case of dihydrotetraazaheptacene (acene backbone), the molecules align in zigzag direction, and the resulting fibers follow an armchair direction of the

substrate. Furthermore, these results indicate that CVD grown MoS₂ grains predominantly terminate by zigzag edges.

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OGD-2 POSTER

TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00

BASEMENT

Materials for inkjet-printing of a transferable organic photodiode on top of commercially available thin, conformable polymer substrates

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This work investigates the fabrication of an organic photodiode on top of a commercially available conformable polymer substrate which would be able to be easily transferred and adhere to different surfaces. Target surfaces for final application include artificial (flat and smooth e.g. glass or even complex and rough, e.g. concrete, paper, plastic etc.) as well as natural ones (e.g. human skin). To achieve this goal available substrates and materials needed to be investigated. Especially the choice of thin, transferable polymer substrates is crucial. Indeed, not only the transferability is important but also their thickness, surface topography, surface wettability, optical properties, as well as their chemical and thermal stability during processing.

We investigated as suitable substrate materials ethylcellulose or polyurethane/allyl resin films (as in two different compositions of decal transfer paper) releasable from a paper support through dissolution of a water soluble sacrificial layer. Moreover, a transparent medical adhesive based on polyurethane has been considered as well and characterized. Top and bottom electrode were ink-jet printed with PEDOT: PSS and reactive Ag-ink respectively. For the photoactive layer a bulk heterojunction blend consisting of a derivative of polythiophene and a fullerene-derivative is investigated, starting from toluene or water solutions. Characterization of all materials included thickness estimation (stylus profilometry), topography (AFM imaging), UV/vis absorption spectroscopy, wettability (contact angle measurements), conductivity (4-point probe).

The function of the photodiode will be characterized under different circumstances, which include dark current, operation upon different illumination conditions, functionality before and after transfer, as well as adhesion and time stability on target surface.

Investigation of structural inhomogenities and photoresponse of CdZnTe and doped ZnTe crystals on the nanometer scale

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Due to the good efficiency and high energy-resolution, Cd_{0.9}Zn_{0.1}Te (CZT) is one of the most suitable materials for room temperature x- and gamma-ray detectors¹. In the field of terahertz detection and spectroscopy, doped ZnTe (ZT) is suitable for applications also due to higher efficiency compared to intrinsic ZT². However, structural inhomogeneities such as Te inclusions, dislocations, and grain boundaries diminish the device performance and need to be studied thoroughly³⁻⁵. A CZT bicrystal was cut from an ingot grown by a modified vertical Bridgman method⁶. The two CZT grains are separated by twin boundaries. Nanometer scale morphological sample characterization by atomic force microscopy revealed at least two crystallographically different twinning systems. Electron backscattering diffraction (EBSD) and infrared imaging confirmed that the main twinning system is the well-known coherent $\Sigma = 3$, {111} – {111} system. There are steps in the twin plane which can only be described by addition of the lateral {112} – {112} twinning⁷. Morphological considerations of the bicrystal suggest even a third type of grain boundary.

Moreover, the effect of different doping (V, Mn, In) on the photoresponse of ZT crystals grown by temperature gradient solution growth method⁸ was investigated by photoassisted Kelvin probe force microscopy (KPFM), and the involved time constants were determined.

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Modeling metal/self-assembled monolayer interfaces using density functional theory

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Self-assembled monolayers (SAMs) of organic molecules covalently bonded to surfaces are widely used for numerous technological applications in many research areas, in view of their ability to modify surface and interfacial properties. In the increasingly growing field of organic electronics, SAMs are mostly employed to tune carrier injection/extraction barriers from the metal electrode to

the (organic) semiconductor layer, being therefore particularly useful for devices such as organic thin film transistors (OTFTs).

The inclusion of SAMs in real devices, however, requires deep understanding and detailed characterization of the metal/SAM interface. In this regard, quantum mechanical simulations are an extremely powerful tool that allows investigating the systems of interest up to the atomistic level.

In this contribution I give some examples of how density functional theory (DFT) calculations, applied together with periodic boundary conditions and the repeated slab approach, can be used to characterize such interfaces. The electronic and structural properties of the systems are investigated, in order to precisely correlate the specific molecular building blocks to the induced surface modifications. The comparison of calculated and experimental results is discussed as well, emphasizing the importance of combining calculations and experiments for an exhaustive understanding of material properties.

In particular, originally designed dithiocarbamate (DTC) and triptycene based SAMs bonded to coinage metal substrates are considered, which have the peculiarity of adsorbing on the surfaces in a bidentate and tridentate fashion, respectively. Such unconventional docking groups represent new promising platforms for surface modifications.

OGD-5 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Porous silicon based broad-band SERS substrates

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In the last decade surface enhanced Raman scattering (SERS) has become a utilizable, fast, highly sensitive and non-destructive characterization method for research and industry (e.g. as biosensors, for life science applications).

The benefit of high enhancement factors of SERS substrates originates from using plasmonic nanostructures. The effect can be separated in the electromagnetic enhancement generated from localized surface plasmon resonances, which provides the major contribution, and the chemical enhancement related to charge transfer interactions of analyte and plasmonic nanoparticles. The enhancement can furthermore be boosted by using very close nanoparticle arrangements leading to couplings of localized surface plasmon resonances, so called hot spots.

In this study the advantage of a chaotic approached broad-band SERS substrate type, meaning all degrees of freedom regarding spatial formation and arrangement, is shown. These substrates were used to detect different commonly used analytes (e.g. Rhodamine 6G, 1,4-BDT, etc.) with laser excitation wavelengths of 455 nm, 532 nm and 785 nm. First measurements have been performed using analyte concentrations of 1 mM. The substrates are based on arbitrarily arranged porous silicon particles, on top of which silver nanoparticles of different and arbitrary sizes and shapes are randomly grown. This creates a vast variety of SERS active arrangements generating at each excitation wavelength a homogenous and narrow distributed, but different Raman scattering enhancement across the whole surface.

Bio-foam adsorbents used as SERS sensors for detection of low concentrated pollutantsA. Reyer¹, M. Musso¹, N. Cefarin², J. F. Wendisch¹, G. Tondi³, L. Vaccari², G. Bourret¹¹*Department Chemistry and Physics of Materials, University of Salzburg, Salzburg, Austria*²*Elettra-Sincrotrone Trieste, Basovizza/Trieste, Italy*³*Forest Product Technology and Timber Construction Department, Salzburg University of Applied Sciences, Kuchl, Austria*

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Totally natural rigid foams derived from byproducts of wood industries, like tannin-based rigid foams, are innovative materials made of inexpensive organic ingredients, and are produced via an acid catalyzed polycondensation reaction between furfuryl alcohol and condensed flavonoids (e.g. Mimosa tannin).

A possible application of these tannin foams, next to insulating material purposes in green building technology, is their use as adsorbents for wastewater treatment. Biological and chemical contamination of groundwater and wastewater is a widespread problem with the current need of mostly complex (wet-chemistry) analytics to identify the source of contamination. A material acting as both adsorbent and sensor for detecting low concentrated pollutants in a fast and easy way would be a huge benefit.

Surface-enhanced Raman scattering (SERS) is a suitable spectroscopic technique for this challenge, being a non-destructive and rapid method for detecting substances even down to trace analysis level, without requiring biomarkers or long incubation times as usually needed for fluorescence spectroscopy or microbiological investigations. The creation of reliable SERS substrates usable for specific applications has been in focus of intense research since many years.

In our approach tannin-based bio-foams are functionalized with noble metals to create localized surface plasmon resonances (LSPR). After contamination with some specific, highly diluted target molecules, this yields a SERS signal in the visible and NIR spectral range. First steps in the direction of future applications for waste-water and environmental diagnosis are forecasted.

This research is part of the Interreg Italy-Austria ITAT1023 InCIMA project funded by the European Regional Development Fund and Interreg V-A Italy-Austria 2014-2020.

Growth and structure of molybdenum oxide layers on Pd(100)

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Molybdenum trioxide (MoO₃) exhibits photochromic and electrochromic properties, and is thus of potential interest for displays and smart window devices. Due to its high dielectric constant, MoO₃ may serve as an ideal gate dielectric for atomically thin transistors based on two-dimensional (2D) semiconductors. Hence, fabricating MoO₃ in a 2D form is of great technological importance. Here, we investigate by scanning tunneling microscopy (STM) and low electron energy diffraction (LEED) the growth and surface structure of ultrathin MoO₃ films on a single crystal Pd(100) surface.

MoO₃ has been deposited by physical vapor deposition of MoO₃ powder from an electron beam evaporator onto the clean Pd(100) surface at room temperature, followed by post-oxidation annealing at 400°C in an oxygen pressure of 2×10^{-6} mbar. At low oxide coverage (< 0.5 ML), STM images reveal

open labyrinth-like structures, which exhibit a poor long-range order. With increasing the coverage more compact oxide islands form, which display a $c(2 \times 2)$ periodicity. At ~ 1 ML the $c(2 \times 2)$ islands arrange in a nanoscale domain pattern of antiphase domain boundaries, very similar to that observed in a 2D WO_3 layer on Pd(100) [1]. The latter has been assigned with a 2D sheet of a cubic WO_3 bulk structure. Above 1 ML, the growth of second layer islands take place with an apparent height of 6\AA , which is compatible with the separation of (010) bi-layer sheets in the bulk $\alpha - \text{MoO}_3$ phase. This indicates that already the second MoO_3 layer on Pd(100) mimics the bulk oxide structure.

This work has been supported by the FWF Project P26633-N20.

[1] N. Doudin, D. Kuhness, M. Blatnik, G. Barcaro, F. R. Negreiros, L. Sementa, A. Fortunelli, S. Surnev, F.P. Netzer, *J. Phys. Chem. C* **120** (2016) 28682-28693.

OGD-8 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Na doping of a WO_3 monolayer on Ag(100): Formation of 2D Na_xWO_3 bronzes?

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The tungsten bronzes are non-stoichiometric tungsten oxides of the form M_xWO_3 , where $0 \leq x \leq 1$ and M is a dopant ion, usually an alkali metal, most commonly Na. By varying the Na content in Na_xWO_3 , substantial changes in the electrical and optical properties of the material are observed. Studies of structurally well-defined surfaces or thin films of Na_xWO_3 are however scarce. Here we investigate the feasibility of fabricating this interesting material in the form of a two-dimensional (2D) layer. The preparation approach consists of the deposition of cyclic $(\text{WO}_3)_3$ clusters, obtained by sublimation of WO_3 powder in a thermal evaporator, onto a Ag(100) surface held at 500°C , which results in a compact and epitaxial WO_3 overlayer [1]. Subsequently, Na metal has been deposited from a commercial SAES getter source onto the WO_3 layer at room temperature.

The doping of the WO_3 layer with Na has been characterized by x-ray and ultraviolet photoelectron spectroscopies (XPS and UPS), and low-energy electron diffraction (LEED) measurements. The deposition of ~ 0.5 ML of Na results in a decrease of the WO_3 work function from 5.8 eV to 3.6 eV, indicating a significant charge transfer from the Na atoms to the WO_3 layer. This is also in line with the $\text{NaKL}_{23}\text{L}_{23}$ Auger spectra, which show a peak with a kinetic energy of 990 eV characteristic of ionized Na species. Corresponding changes have been observed in the oxide W 4f and O 1s XPS spectra, suggesting that the Na atoms are reacting with the WO_3 layer. LEED measurements indicate the formation of ordered structures, which will be investigated in more detail in STM.

This work has been supported by the FWF Project P26633-N20.

[1] T. Obermüller, N. Doudin, D. Kuhness, S. Surnev, F. P. Netzer, *J. Mat. Res.* **32** (2017) 3924-3935.

Molecular motors on Cu(111) studied by scanning tunneling microscopyM. Schied¹, P. Jacobson¹, D. Liu², J. M. Tour², L. Grill¹¹*Institute of Physical Chemistry, University of Graz, Austria*²*Department of Chemistry, Rice University, USA*

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Artificial molecular motors can translate an external stimulus into controlled motion. They have seen great developments in the last decades [1]. While many studies exist in solution, only very little is known how such functional molecules behave on a surface, although such a setup holds the advantage of a fixed point of reference. This is of importance for a key property of molecular machines, the directionality of their motion in a static environment. In this study, artificial motor molecules have been investigated, all based on a combination of double bond isomerization and helix inversion, which are the key processes responsible for rotation of the so-called Feringa motor. This type of motor has already been used to successfully drive lateral translation of molecules at surfaces [2, 3]. Experiments were done by low temperature scanning tunneling microscopy (STM) to enable imaging of one and the same molecule before applying an external stimulus. The focus of our study is on the adsorption of such molecules at metallic surfaces and what type of motion can be induced by either STM manipulation or illumination by light.

[1] W. R. Browne and B. L. Feringa, *Nat. Nanotech.* **1**, 25 (2006)[2] T. Kudernac *et al.*, *Nature* **479**, 208 (2011)[3] A. Saywell *et al.*, *ACS Nano* **10**, 10945 (2016)**Growth morphologies and thermalization pathways of nitrogen based oligoacene derivatives on (0001) sapphire**A. Çiçek¹, Matković¹, M. Kratzer¹, Z. Chen², O. Siri², C. Becker² and C. Teichert¹¹*Institute of Physics, Montanuniversität Leoben, Leoben, Austria*²*Aix Marseille Univ., CNRS, CINaM, Marseille, France*

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Oligoacenes (as pentacene) and their derivatives are considered as potential candidates in the field of organic electronics due to their molecular packing that favours charge transport and thus high field-effect mobilities. Here, dihydro-tetraaza-pentacene (DHTA5) and dihydro-tetraaza-heptacene (DHTA7) molecules are considered [1,2]. Both molecules exhibit a similar dipolar momentum and hydrogen bonding in the crystal, but have a different size of the backbone. Molecular arrangement, nucleation densities, sizes, and shapes of the resulting crystallites are analyzed as a function of the deposition temperature [3].

The molecules are deposited using a hot wall epitaxy system. As substrate, vicinal (0001) sapphire is used with an average step distance of 50 nm, and step height of 0.2 nm. The morphology of the grown films is investigated ex-situ by atomic force microscopy. Coverages from sub-monolayers to several layers are analysed, and evolution of needle-like and island-like crystallites is examined as a function of the deposition temperature. An activation energy of (1.23 ± 0.12) eV was found for the nucleation of DHTA7 islands (composed of upright standing molecules), while (1.16 ± 0.25) eV was obtained for DHTA5 needles (composed of lying molecules). The observed disparity in the temperature dependent nucleation densities of the two molecular species is attributed to the different thermaliza-

tion pathways of the impinging molecules [4].

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[3] A. Matković, A. Çiçek, M. Kratzer, B. Kaufmann, A. Thomas, Z. Chen, O. Siri, C. Becker, and C. Teichert, *Surface Science* (2018), <https://doi.org/10.1016/j.susc.2018.03.009>.

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OGD-11 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

DHTAP thin layers deposited on Cu(110) and Cu(110)-(2 × 1)O surfaces

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Dihydrotetraazapentacene (DHTAP) is a derivate of pentacene, which due to its two H-donor (N-H) and the two H-acceptor (N=C) sites, is expected to form well-ordered molecular structures on surfaces. Here, we study the morphology and the evolution of the optical properties during the deposition of DHTAP thin layers on Cu(110) and Cu(110)-(2 × 1)O surfaces using polarization-dependent differential reflectance spectroscopy (pol-DRS)[1] in combination with photoelectron emission microscopy (PEEM). We compare our results to those obtained by in situ reflectance differential spectroscopy (RDS) in a second experiment. Within the first monolayer, DHTAP adsorbs in a flat-lying geometry on both surfaces. However, the orientation of the long molecular axis of the molecules in the first monolayer is aligned along the [1-10]-direction on the Cu(110) surface, while it is parallel to the [001]-direction on Cu(110)-(2 × 1)O. We find that, depending on the growth temperature, the DHTAP molecules on top of the first monolayer deposited on Cu(110) change their preferential alignment.

[1] A. Navarro-Quezada *et al.*, *Rev. Sci. Instr.* **86**, 113108 (2015)

OGD-12 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Evaluating different Models for the Analysis of Tunneling Current-Voltage Curves in Metal-Molecule-Metal Molecular Junctions

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When characterizing molecular and monolayer junctions one of the key-parameters used is the so-called transition voltage. Unfortunately, its relation to the intrinsic electronic properties of the

junction is still poorly understood, although Baldea, Frisbie and co-workers have recently obtained an excellent correlation between the energetic positions of the electronic transport channels extracted from a simple one-state model and the positions of the peaks in the density of states obtained via photoelectron spectroscopy measurements.

This raises the question, to what extent a model building on a single, discrete energy level can be sufficient to represent the complex electronic structure of the junction. We investigated the applicability of the aforementioned model especially in view of the vastly different coupling strength between substrates and molecules upon changing the docking chemistry.

For this, we simulated the electronic structure of a wide range of molecular junctions using density functional theory based methods and calculated the current-voltage characteristics by employing the Landauer-Büttiger formalism. Finally, from these characteristics we fitted the energetic position of the above-mentioned discrete "transport" level. Its properties are then compared to the actual electronic structure of the junction.

OGD-13 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Photochemical switching of azobenzene derivatives on an insulating surface

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Studying single molecular switches is of interest for a better understanding of fundamental physical and chemical processes, but also in view of their possible use in molecular nanotechnology [1]. A prototypical conformational switch is azobenzene, which changes between *trans* and *cis* isomers at the central N=N bond upon an external stimulus, showing efficient photochemical activation. In the past years, various studies have shown that adsorption on metal substrates strongly influences the switching properties [2,3], especially for activation by light [4]. We present non-contact atomic force microscopy (nc-AFM) results on the switching of individual azobenzene molecules on a calcite surface where the molecules retain their photochemical activity.

[1] C. Joachim *et al.*, *Nature* **506**, 651 (2000)

[2] Choi *et al.*, *Phys. Rev. Lett.* **96**, 156106 (2006)

[3] Dri *et al.*, *Nature Nanotechnology* **3**, 649 (2008)

[4] Comstock *et al.*, *Phys. Rev. Lett.* **99**, 038301 (2007)

OGD-14 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

The Interface of Coronene with the (111)-Surfaces of the Coinage Metals: Geometry and Electronic Structure

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As a first step we have determined the most favorable adsorption sites and molecular orientations based on the experimentally known over-layer structures. The systems show a flat adsorption geometry and a common azimuthal molecular orientation that is - particularly for the case of Ag(111) - in good agreement with the experimental orientation. For the copper surface, additional calculations with a hybrid functional were utilized to clarify the HOMO position. For the case of gold we furthermore investigated the impact of different van der Waals treatments on the adsorption geometry.

In a second step, we have simulated angle-resolved photoemission spectroscopy (ARPES) experiments for coronene on the three coinage metal (111)-surfaces, focusing on the emissions from the HOMO. Simulated photoelectron angular distributions (PADs) for the coronene/metal interfaces show pronounced differences to PADs of the two-fold degenerate HOMO of the isolated molecule. We conclude that the observed symmetry-breaking results from the molecule-substrate-interaction and intermolecular band dispersion. The observed sub-structure of the major emission features in the PADs compares well to the experimental findings which were available for (111)-Ag [1].

[1] Udhardt, C.; Otto, F.; Kern, C.; Lüftner, D.; Hümpfner, T.; Kirchhübel, T.; Sojka, F.; Meißner, M.; Schröter, B.; Forker, R.; Puschnig, P. & Fritz, T., *J. Phys. Chem. C* **121**, 12285-12293 (2017).

OGD-15 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Growth of small organic molecules on ultrathin hexagonal boron nitride

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The role of ultrathin, two-dimensional (2D) substrates in the development of novel electronic devices is yet to come. Quasi 2D materials can act as optically transparent and mechanically flexible electrodes or dielectrics in organic electronics. Graphene as potential electrode material has been studied to some extent as substrate for organic thin film growth [1-5]. Besides graphene, hexagonal boron nitride (hBN) has come into the focus of research as an ultra-thin dielectric. Here, we present the study of growth morphologies of the non-polar small organic model molecule para-hexaphenyl (6P) [6] as well as of the polar dihydrotetraazaheptacene (DHTA7) on SiO₂/Si supported, exfoliated hBN. The substrates have been prepared by micromechanical exfoliation from hBN powders and subsequent transfer to SiO₂/Si substrates. The organic thin films have been deposited by means of hot wall epitaxy in a temperature range between room temperature and 360 K. The resulting morphologies were characterized ex-situ by means of atomic force microscopy. The main growth features are crystalline needle networks that exhibit clear epitaxial relationships between substrate and organic crystal. Comparison with density functional theory (DFT) calculations revealed a (-629) contact plane between 6P and hBN. This resulted in a splitting of $\pm 6^\circ$ of the needle growth directions to the hBN zig-zag orientation. For the acene-like DHTA7, very long needles with a splitting of $\pm \sim 9.5^\circ$ with respect to the armchair direction has been found.

[1] G. Hlawacek *et al.*, *Nano Lett.* **11**, 333 (2011)

[2] M. Kratzer *et al.*, *J. Vac. Sci. Technol. B* **31**, 04D114 (2013)

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[5] A. Matković *et al.*, *Sci. Rep.* **7**, 46794 (2017)
[6] A. Matković *et al.*, *Sci. Rep.* **6**, 38519 (2016)

OGD-16 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Spectroscopic Investigation of Catechol on Iron Oxides

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Catechol, an organic molecule consisting of a benzene ring with two OH groups in ortho position, is a compound in the production of pesticides and plays an important role in bio-oil production. It is also a natural component of plants, fruits and vegetables, thus occurring also in soil, where it is often exposed to iron oxides, which are abundant in nature. Therefore, we investigated the behaviour of Catechol in contact with iron oxides to aid in the understanding of the involved adsorption and degradation processes. For this task, we prepared model systems by growing FeO, and Fe₃O₄ epitaxially on a Pt(111) single-crystal in UHV conditions. Catechol was then deposited by background dosing on pristine Pt(111), FeO and Fe₃O₄ at liquid nitrogen (LN₂) sample temperature. Subsequently, Fourier-Transform Infrared Reflection Absorption Spectroscopy (FT-IRAS) and Scanning Tunneling Microscopy (STM) were performed to investigate the adsorption behaviour. For the characterization of the chemical structure we conducted XPS measurements. Furthermore, temperature series were performed in order to study the stability and reactivity of the adsorbed molecule. For this purpose we additionally employed Temperature Programmed Desorption (TPD) series.

On this poster we present our findings on the desorption as well as the decomposition behaviour on before mentioned substrates. Additionally, a model for the adsorption of the monolayer of Catechol is proposed.

OGD-17 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

The electronic structure of a monolayer C₆₀/Ag(110) investigated by density functional calculations and photoemission spectroscopy

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We employ density functional theory (DFT) calculations to determine the preferred adsorption geometry of a monolayer C₆₀ on the Ag(110) surface. The analysis of the electronic structure reveals a partial occupancy of the LUMO of C₆₀ upon adsorption, where the interaction with the substrate lifts the degeneracy of the LUMO states. To further study the electronic structure of the C₆₀ layer, we simulate photoelectron angular distributions (PADs) of the HOMO and the LUMO initial states of gas phase C₆₀ as well as of the C₆₀/Ag(110) interface. The final state of the photoemission process is either treated as a simple plane wave, an approach which has proven very successful for various planar-conjugated molecules, or by using the more sophisticated independent atomic

center (IAC) approximation which can also account for scattering effects of the outgoing electron. The comparison of simulated with measured PADs confirms the adsorption geometry predicted by DFT. Moreover, the comparison between the plane wave and the IAC results allows us to quantify the importance of scattering effects in the theoretical description of photoemission for non-planar molecules.

OGD-18 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Epitaxial Order of Pentacenequinone Films on Graphene and Au(111)

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The formation of epitaxial order is studied for pentacenequinone (P2O) thin films with a nominal thickness of approximately 3.5 nm. Films were prepared by physical vapor deposition under ultra-high vacuum conditions on a Au(111) surface and on top of a graphene monolayer prepared at a silicon carbide substrate. The deposition process was monitored using differential reflectance spectroscopy starting from the bare substrate up to approximately 10 monolayers of coverage. Indexation of the low energy electron diffraction (LEED) measurements successively allowed the determination of the crystallographic unit cell of the adsorbate layer and its epitaxial relationships to the substrate. In a subsequent step the epitaxial order of P2O crystallites is investigated by grazing incidence X-ray diffraction (GIXD). The three-dimensional crystal structure can be determined from these measurements by presenting reciprocal space maps and pole figures. Results obtained for P2O on Au(111) and graphene (see Figure 1) show two different surface unit cells as obtained from LEED images. GIXD measurements confirm the appearance of two different crystal structures (cf. Figure 1). One is the known bulk phase [1], the other one the recently reported surface-induced phase of P2O on graphite [2]. This work shows the combination of different experimental approaches to study epitaxy in films ranging from the monolayer regime up to thick films.

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OGD-19 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

The geometric and electronic structure of tetracene/Ag(110) investigated by density functional theory and photoemission experiments

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Tetracene is an organic semiconductor with promising application as an active layer in organic field effect transistors. Since the substrate/molecule interaction plays an important role for determining its electronic properties, it is important to know the structure of the molecule on the substrate. In a recent study, photoemission tomography experiments together with density functional theory were used to determine the structure of tetracene on Ag(110). The origin of two distinct emissions

separated by 1 eV, both appearing to have the photoemission distributions of the highest unoccupied orbital, emerged as an open problem. One proposed solution suggests that the unit cell contains two molecules, where the two molecules occupy different adsorption sites leading to an energetic splitting of the electronic states. In this study we investigate this proposition further by determining the projected density of states of various geometries with alternating molecule-substrate height and by comparing them to the experimental findings.

OGD-20 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Simulating Charge Transport Through Metal-Organic Semiconductor Interfaces: Bulk or Contact Limited?

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In organic electronic devices, contact engineering has become an important field of research. Efficient charge injection is crucial for a decent device performance of, e.g., organic thin film transistors or organic light emitting diodes. Experimentally, the injection process can be influenced by a huge variety of measures to tune interfacial properties like level alignment and disorder. Nevertheless, the complex interplay of those interfacial properties and their impact on the bulk current is only poorly understood from a theoretical point of view.

To overcome this lack of knowledge, we utilize mesoscopic simulations to predict the current across the contact interface under operation. In these simulations, charges are viewed to migrate through disordered organic semiconductors due to hopping between localised states. Parameters like injection barrier, energetic disorder, electric field, Coulomb interactions and temperature can be directly considered. This intuitive method to describe the hopping of charges holds the promise to understand the effects and interactions that govern the interplay between interfacial and bulk properties. So far, the interpretation of the interface current in terms of local charge densities has been impaired by a highly simplified consideration of the contact. By reformulating the contact description, we enable a straight-forward interpretation of the current.

Based on the improved contact description, we analyse the current density across the contact interface and in the bulk for instructive combinations of interface and bulk properties. This analysis yields two distinct regimes, a bulk limited regime and a contact limited regime. The evolution of the current density with respect to the injection barrier, the energetic disorder and the electric field strength is thoroughly investigated and the origin of bulk vs. contact limitation is analysed.

OGD-21 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Organic Molecules on Alkali Halide and Metal Oxide Interlayers: A Characterisation of Energy Levels and Charge Transfer

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For organic devices, thin layers of alkali halides or metal oxides at the electron injection contact are seen to improve their characteristics. Previously, “trial and error” methods were used to facilitate desirable properties such as better electron injection. Technological progress and new experimental tools answered many questions, however, the discussion on specifics concerning orbital level alignment and charge transfer is still open.

In this work, charge transfer across interlayers was investigated using photoemission tomography (PT) with angular resolved photoemission spectroscopy (ARUPS). PT provides compelling evidence of molecular geometries, number of charged molecules and links orbitals with specific emissions. Here, the “big five” factors governing charge transfer are surveyed: dielectric work function, dielectric thickness, interlayer polarisability, electron affinity and molecular geometry. On silver, films of magnesium oxide (MgO) (100) and potassium chloride (KCl) (100) are grown and exposed to para-sexiphenyl (6P) and pentacene (5A). On both the KCl and MgO interlayers charge transfer occurs and the number of charged molecules could be controlled. The principle factor in both cases is the interlayer work function. However, it is shown that at the atomic level, the mechanism is significantly different on the two dielectric films. For MgO, it is governed by defects at the MgO/Ag interface, while for KCl it is by defects on the outer surface.

OGD-22 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Methodology of Crystal Structure Determination for Thin Film Phases

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A change in the structural order of organic molecular crystals is observed often for films, that are thin enough to interact strongly with the substrate, they are grown upon. New polymorphic phases can be accessed this way, known as substrate-induced phases (SIPs), the most prominent example being pentacene. The structure solution of such phases is challenging, as there are no well-established methods like when dealing with crystalline powders or large single crystals. A combined approach of using grazing incidence x-ray diffraction (GIXD) to measure and index the Bragg peaks as well as computational refinement with methods like molecular dynamics (MD) simulations, to determine the exact packing, is a promising methodology. One set of samples are molecular crystals of 2-decyl-7-phenyl-[1]benzothieno[3,2-b][1]benzothiophene (Ph-BTBT-10). Thin films are prepared by physical vapour deposition and by spin-coating from toluene solutions on silicon oxide surfaces. Additionally, a mixed crystal film from p-sexiphenyl (6P) and α -sexithiophene (6T) deposited onto silicon as well as highly oriented pyrolytic graphite (HOPG) is studied.

Predicting and understanding surface polymorph formation of acenequinones on Ag(111) using the SAMPLE approach

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A variety of properties of metal-organic interfaces are determined by the polymorph that the molecules assume on the (metal) surface. In order to engineer functional interfaces, it is therefore imperative to predict which polymorphs form for a given material combination. Still, there are surprisingly few systematic studies that allow inferring reliable relationships between the molecular structure and the kinds of interface polymorphs that form. This is because experimentally, the vacuum deposition of molecules often leads to kinetically trapped phases. Conversely, computational studies are hindered by the intractably vast number of possible polymorphs, also known as “configurational explosion”.

In this contribution we computationally investigate the formation of surface polymorphs on the example of acenequinones on Ag(111). We perform an exhaustive structure search utilizing the SAMPLE¹ approach. It first performs a physically-motivated coarse graining of the configurational potential energy surface to generate an exhaustive set of polymorph candidates. To overcome the configurational explosion a machine learning model in the form of Bayesian linear regression is trained on a small subset of possible polymorphs and then used to predict the adsorption energies of all of them. This method allows us to find the low energy polymorphs and surface patterns of different acenequinones. For those patterns we can further explain the driving forces for their formation by dividing the formation energy into molecule-substrate and molecule-molecule contributions.

[1] M. Scherbela, L. Hörmann, A. Jeindl, V. Obersteiner and O.T. Hofmann, *Physical Review Materials* **2** (4), 043803

Tuning the Charge Transfer at Hybrid Interfaces: F4TCNQ on ZnO

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At inorganic/organic hybrid interfaces, charge transfer occurs in different forms depending on the nature of the substrate. On metals, where the adsorbate often hybridizes with the substrate, hybrid bands are formed. These lead to a uniform, fractional charging of the organic molecule. In contrast, on insulating, inert substrates, charge is transferred as integer electrons, which leads to the coexistence of charged and neutral molecules on the surface. This raises the question which property - the hybridization or the abundance of charge carriers - is the cause for the different mechanism.

To answer the question we study the charge distribution of F4TCNQ on different ZnO surfaces using hybrid density functional theory. ZnO is a particularly interesting substrate, as it can be produced with high purity, making it basically insulating, or it can be doped until it shows metallic conductivity. Employing a recently developed approach to incorporate doping and the effect of long-ranged band bending into our calculations, we investigate the charge transfer mechanism over a large range of doping concentrations. Furthermore, to study the impact of hybridization we employ two different surfaces of ZnO: The O-terminated (000-1) surface is inert due to the presence of a hydrogen over-

layer, while the mixed-terminated (10-10) surface exposes surface Zn atoms that can hybridize with organic adsorbate. We find that the doping concentration only affects the amount of charge transferred, but not the mechanism. At the same time, we find that due to hybridization on the mixed-terminated surface, a previously not described coexistence of integer and fractional charging is observed.

OGD-25 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Fast Low-Noise Current Preamplifier for Scanning Tunneling Microscopy

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Scanning tunneling microscopy is one of the most versatile techniques for the analysis of surface properties. One of the factors limiting its performance is the bandwidth and noise of the preamplifier. Higher bandwidth enables faster scanning, with the advantages of better time resolution, larger undisturbed image areas between tip changes. A high bandwidth also implies low phase shifts, which reduces the susceptibility to feedback loop oscillations.

STM preamplifiers are current-voltage converters (transimpedance amplifiers), usually with a high feedback resistor. Increasing resistor values leads to lower current noise (Johnson noise) introduced by the resistor, but at the same time usually results in lower bandwidth. Typical values for commercial STM amplifiers are about 20-80 kHz bandwidth and $\leq 20 \text{ fA}/\sqrt{\text{Hz}}$ RMS noise. Using a multi-stage amplifier design, we could achieve an input noise below $10 \text{ fA}/\sqrt{\text{Hz}}$ at low frequencies, but nevertheless a high bandwidth of 250 kHz, much larger than that of most commercial low-noise preamplifiers.

We also demonstrate that minimizing the input capacitance is of paramount importance for low noise. This means that connecting the STM tip to the preamplifier via a long coaxial cable is unfavorable, and the performance can be substantially improved by placing the first amplifier stage into vacuum. Additionally, for low-temperature STMs, the Johnson noise of the feedback resistor can be reduced by placing it in thermal contact with the cryostat.

OGD-26 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Ultrathin, adhesive ink-jet printed skin-contact electrodes

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Organic and printed electronics is enabling novel sensing technologies especially in the field of wearable/skin-contact biomedical devices. Ink-jet printing of conducting polymers on top of suitable thin substrates has been explored for developing skin-contact electrodes. These are used as sensors for physiological monitoring like Electrocardiography (ECG) or Electromyography (EMG). Our approach focused on “smartening” commercially available materials like transparent medical adhesives, with the objective of creating a robust while lightweight and unperceivable electrical interface with skin. For this we investigated the electrical, mechanical and optical properties of a conductive polymer ink - a dispersion of poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT:PSS)- on the different suitable transferrable substrates. Furthermore, it was shown that it is

possible to retrofit materials with a working inkjet printed ECG/EMG electrode and record data with it.

One of the main challenges in so-called “epidermal electronics” is to provide a good electrical connection from the ultrathin/conformal sensor to an external recording device. In order to address this issue, methods including pyrolyzation + deposition of conductive polymer were investigated to provide Vertical Interconnect Access (VIAs) for future multilayer circuits.

Due to the application skin-electrodes undergo repeated mechanical stress such as stretching and compressing. To simulate this stress a mechanical setup was designed and the mechanical + electrical properties of the electrodes were investigated.

OGD-27 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Methanol adsorption and decomposition on mixed CuO - CuWO₄ surfaces and a WO₃ monolayer

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We investigate the chemical reactivity of a newly found ultrathin 2D WO₃ nanolayer on Pd(100) and mixed, ultrathin 2D CuO - CuWO₄ surfaces on Cu(110), with coverages between 0 and 1 ML. These were studied as model catalyst systems towards adsorption and reaction of methanol (CH₃OH) using a combination of high-resolution XPS, LEED, STM, HREELS and TPD. While the WO₃ film consists of a bilayer formed by a WO₂ sheet and a terminal tungsten O atom, the ternary CuWO₄ oxide can be described as a trilayer arrangement of tetrahedrally bound W atoms terminated by Cu-O rows. On the ternary CuWO₄ oxide layer methanol has been dosed at 110 K where it adsorbs molecularly as a multilayer. Upon heating to higher temperatures, first a transformation to a methanol monolayer, dehydrogenation to methoxy (CH₃O) and some formaldehyde (CH₂O) intermediates and formation of hydrocarbon (CH_x) adsorbates has been observed. For mixed CuO - CuWO₄ oxide surfaces with coverages between 0.65 ML and 0.8 ML, heating to 450 K has not lead to complete desorption of the methoxy species as for other coverages. These mixed surfaces show the largest methoxy yield and degree of reduction. This strongly indicates that the oxidation reaction is promoted at the periphery of the oxide islands, which expose a large number of active under-coordinated reaction sites. STM measurements confirmed an initiated methanol oxidation reaction at the CuO - CuWO₄ island boundary. Dosing methanol on the 2D WO₃ nanolayer at 110 K results in the formation of a methanol monolayer and some methoxy intermediates. However, no formation of formaldehyde intermediates is observed. The presence of terminal O vacancies, obtained via a formation in a more reducing environment, leads to a higher formation of methoxy species. Both surfaces can be restored into their pristine state by a treatment in oxygen.

Surface analysis of Molybdenum nanoparticle films by SPM

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By scanning tunneling microscope (STM) and atomic force microscope (AFM) we analyzed films of molybdenum that are formed via DC magnetron sputtering. By ionizing argon atoms and accelerating them towards a molybdenum target, molybdenum atoms leave the surface and cover the substrate. In our experiments we deposit the nanoparticles on to highly orientated pyrolytic graphite (HOPG). The size, shape and behavior of the molybdenum nanoparticles are investigated as a function of plasma parameters.

This work was supported by the FWF (Project numbers P26635, P31149 and W1259), and EFRE K Regio Faenomenal.

Correlation length and dimensional cross-over in a quasi-one-dimensional surface system

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The strongly anisotropic adsorbate system Br/Pt(110) exhibits an anomalous order-order phase transition due to competition between inter-adsorbate repulsion and charge density wave (CDW) correlations. The phase transition is preceded by fluctuations between a normal $c(2 \times 2)$ adsorbate phase on a flat surface and a (2×1) phase involving a periodic lattice distortion of the substrate. Here we study the fluctuations, determine the correlation length in reciprocal space and report a novel method for its measurement in real space. Using both methods we study the evolution of the correlation length with temperature. This allows to identify a critical temperature. However, since around the critical temperature the adsorbate mobility freezes out, the transition remains incomplete, resulting in a 2D nematic glass at low temperature. In the temperature range, where the fluctuations occur, the system is demonstrated to be close to a 1D \rightarrow 2D cross over. This unusual phase transition driven by competing interactions exhibits several parallels to phenomena observed in unconventional superconductors.

Hexagonal Boron Nitride: Growth, domain boundaries and defects on Pt(110)

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Hexagonal Boron Nitride (h-BN) belongs to the graphene-class materials, which can be prepared as flat or buckled monatomic layers on diverse substrates and can even be lifted off and transferred to different supports allowing the construction of monolayer stacks. Since h-BN features a large band gap (~ 6 eV), it is well suited for electronic applications in combination with graphene or silicene. If grown on monocrystalline substrates, h-BN usually forms a Moirè pattern which eventually can serve as template for cluster deposition in catalytic applications. Recently, defects in h-BN monolayers were found to act as efficient single photon sources for quantum optical applications.

Using scanning tunnelling microscopy (STM) and low energy electron diffraction (LEED) we study the deposition of h-BN on Pt(110), since we found that this substrate leads to preferential growth of only two 180° rotated domains, in contrast to other supports, where a usually multitude of differently oriented domains is observed. Of particular interest are grain boundaries and defects, because, depending on the substrate, they are chemically active even in the absence of catalyst metals on top of the film. Random defects can be generated by electron or ion bombardment, but we could create a certain type of point defect also by a particular preparation protocol.

OGD-31 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Dynamic *in situ* Observation of Protein Adhesion and Chemical Coupling using Liquid Atomic Force Microscopy

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Protein based bioprocesses are essential for each living organism although complex in their dynamics and final implications. Hence, unravelling their chemical and physical interaction principles is not only important for gaining fundamental understanding but also paves the way for entirely new applications concepts in life sciences. For a long time, electron and / or fluorescence based microscopy have successfully been used for accessing interaction mechanism and their consequences on material systems. However, the former often lacks dynamic studies, while the latter is limited in their lateral resolution. During the last decade, atomic force microscopy (AFM) in liquid environments has attracted significant attention as it enables dynamic studies in close-to-nature conditions with molecular resolution. Furthermore, state-of-the-art AFM instrumentation provide high-speed capabilities with frame rates in the lower second range, which enables true real time studies of bioprocesses such as antibody-antigen interactions or direct protein binding. In this contribution, we apply liquid AFM (L-AFM) for high-resolution studies of thin cellulose films, whose surface is dynamically modified by different proteins, supported by immobilization molecules. While fundamental in this first step, the bigger aim is the fabrication of variable biosensors by using the same platform, equipped with different antibody-antigen coupling for selective sensing.

In more detail, we directly visualize adsorption, chemical bonding and further interaction with appropriate analytes in liquid conditions, complemented by surface plasmon resonance measurements. The findings not only allow specific adaption of the fabrication process but also enable a fundamental insight in cellulose-immobilization molecule-antibody-antigen binding mechanism, barely possible with any other technique on that scale in real time.

PHYSICS-INDUSTRY

(PIN)

PIN-1 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Investigation of selected thermophysical properties of NIST Standard Reference Material 1155a

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The National Institute of Standards and Technology (NIST) provides a multitude of Standard Reference Materials (SRM). These SRMs are widely used as calibration standards and helping tool to develop new measurement methods. In order to take advantage of such a material for calibration purposes or development, it is therefore of great importance to possess accurate data of SRM's properties, including respective uncertainties.

We are studying a selection of thermophysical properties of the NIST SRM stainless steel 1155a (Cr18 Ni12 Mo2) utilizing our ohmic pulse-heating apparatus (OPA), our electromagnetic levitation (EML) apparatus in combination with the oscillating drop (OD) method as well as a commercial differential scanning calorimeter (DSC) NETZSCH 404 C Pegasus.

Measurement with the OPA grants us access to the determination of specific enthalpy, specific resistivity, thermal expansion and density as well as an estimation of thermal conductivity and thermal diffusivity in the solid as well as the liquid phase. Utilizing the EML apparatus gives us the possibility to measure surface tension and density. Specific heat will be measured by means of DSC. All measured data will be provided with uncertainty estimations by means of the Guide to the Expression of Uncertainty in Measurement.

PIN-2 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00 BASEMENT

Density of liquid metals by means of high-pressure ohmic pulse-heating and estimation of critical point data

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Critical point data of high-melting metals are extremely difficult to obtain experimentally due to the enormously high pressure and temperature at this unique point in the phase-diagram. There are, however, extrapolation methods that use the metal's liquid phase density and, according to theoretical models, extrapolate these data to the critical point.

For selected metals, density as a function of temperature was thus measured using an ohmic pulse-heating apparatus. With this method, a large current pulse is discharged through a wire-shaped sample that heats up, expands and finally explodes when reaching the boiling point. During the short

experimental duration of typically $80\ \mu\text{s}$, the temperature is monitored by means of pyrometry and the thermal expansion of the wire is imaged with a special streak camera. This camera takes images of the expanding wire approximately every $2.5\ \mu\text{s}$ and allows to derive density as a function of temperature up to several thousand K above the melting point.

The pulse-heating experiments were conducted under static pressures of up to 3000 bar to increase the boiling point of the sample, and thus obtain data closer to the critical point. These data then serve as input for the estimation of the phase diagram at higher temperatures and consequently the critical temperature and critical density.

The experimental setup and the consecutive data evaluation will be presented. Results for density as a function of temperature and derived critical temperature and critical density will be discussed for selected high-melting metals.

PIN-3 POSTER TUESDAY SEP 11, 17:30-18:30 & WEDNESDAY, SEP 12, 17:30-19:00

BASEMENT

Investigating the Surface Tension of Steels using Electromagnetic Levitation, Part I: Iron-Nickel Alloys

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Surface tension of melts is an important input parameter for simulation tools that are used by today's metalworking industry for describing and optimizing production processes. To obtain valid results from these simulations, accurate experimental data of surface tension and other temperature dependent physical properties, usually termed "thermophysical properties", are needed. But due to the melts high temperatures and chemical reactivity, the measurement of surface tension is a sophisticated task.

The oscillating drop (OD) method in combination with an electromagnetic levitation apparatus (EML) allows to measure surface tension and density of melts in a contact- and container-less manner so that interactions and chemical reactions of the melt with other materials are avoided. Using EML, the liquid sample is levitated freely in space by applying a high-frequency electromagnetic field that exerts a Lorentz-force on the sample, counteracting gravitational force. The OD method is used to relate the observed surface oscillations to the surface tension of the liquid sample.

Our recent experiments examining the influence of the composition in iron-nickel alloys on their surface tension revealed unexpected results. First, our surface tension data were lower compared to the scarce literature data available. Second, samples of different compositions did not show different surface tension values. We hypothesize that our results are due to the "non-academic" purity of our sample material. However, to preclude any errors during data analysis or conduction of the experiments, we decided to conduct reference measurements of the same sample material at the electrostatic levitation (ESL) facility at NASA Marshall Space Flight Center (MSFC). In addition, we attempted to self-fabricate samples of "academic-purity" from high-purity iron-nickel wires and investigated those in the ESL too. The ESL measurement results will be presented and compared to our EML data.

Work funded by the Austrian Research Promotion Agency (FFG), Project "Surfacetension-Steel" (Project-Nr. 855678).

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LIST OF AUTHORS

Abdou J-M, 81
Abele H, 111, 112
Achatz L, 111
Adrien M, 63
Agu M, 24
Aguillon F, 28
Aichhorn M, 44
Aiglinger M, 47
Albertini S, 105
Albu M, 37
Alkofer R, 63–65
Allison W, 90
Ameixa J, 75
Amenitsch H, 45, 49, 115
Amentisch H, 76
Amtmann C, 24
Andrews A M, 33, 34
Andrews M, 36
Antczak G, 90
Aquilanti G, 115
Arndt M, 14, 28, 29
Arnold T, 96
Arrigoni A, 41
Arrigoni E, 70
Arthur-Baidoo E, 75
Assmann E, 44
Atteneder F, 65

Böhm H, 42, 43, 110
Baltuška A, 51
Baroncini M, 92
Bechis I, 88
Beck-Erlach M, 76
Becker C, 122, 123, 125
Bednar T, 23
Bedoya-Martínez N, 41, 105, 106
Beiser M, 33, 34, 36
Belza W, 89
Benedek G, 78
Bergauer T, 56, 60, 113
Berger T, 87
Bertel E, 133
Besser B P, 69
Bianchi M, 78
Bieser H, 98
Blöch D, 60
Blatnik M, 132
Boatner L A, 77

Bobek J, 131
Bockstedte M, 44
Bockstedte M, 88
Boese A D, 90
Bogar M, 115
Boisen A, 45
Boné T, 128
Bonanni A, 47
Bosina J, 111
Bourret G, 48, 107, 120
Bourret G R, 36
Brand C, 28, 29
Braxmeier S, 46
Breitegger P, 128
Brondolin E, 59, 112
Budai J, 52
Bulanov S, 53
Burian M, 115
Burker A, 56, 113
Burns C, 119
Burtscher B, 117
Butej B, 86

Campi D, 78
Capeta D, 116
Cartus J J, 101
Cefarin N, 48, 107, 120
Cesnik S, 29
Charalambidis D, 50, 51
Chen Z, 122, 125
Cheng H-W, 93
Christian P, 94
Çiçek A, 122
Civita D, 91
Coclite A M, 79, 80, 94
Contant R, 64
Credi A, 92
Cronenberg G, 111
Czibula C, 40

D'Amico F, 48, 107
Dürrbeck S, 133
dal Cin S, 33
Dallinger A, 131
De Franco A, 113
Debiossac M, 28
Denifl S, 75
Denoth A, 67
Detz H, 33, 34, 36

Devreese J T, 35
 Diebold U, 77, 80
 Dienstleder M, 110
 Dietl T, 47
 Dirin D, 46
 Diwald O, 36, 87
 Dluzewski P, 47
 Dombi P, 51, 52
 Domke J, 127
 Donati F, 20
 Donato S, 48, 107
 Dong J, 118
 Dorda A, 41
 Dorn G, 70
 Doudin N, 132
 Dragicevic M, 60
 Drechsel C, 102, 132
 Dreossi D, 48, 107
 Dri C, 84
 Durstberger-Rennhofer K, 111

Eadie A, 36
 Ebner C, 38
 Eckert J, 38
 Egger A T, 85, 86, 130
 Egger L, 87, 127
 Ellis J, 90
 Ellmeier M, 24
 Emhofer J, 22
 Enzinger R, 39
 Erker S, 130
 Ernst W E, 26, 27, 29–32, 78, 82, 83, 90
 Escher B, 38

Faina B, 47
 Farka D, 93
 Feng Z, 84
 Ferreira da Silva F, 75
 Feyer V, 84
 Fiala R, 115
 Filter H, 111
 Fink J M, 19
 Fisslthaler E, 110
 Fitzek H, 83, 108
 Foelsche U, 69
 Forker R, 124
 Franchini C, 35
 Fritz T, 124, 127
 Fuchsberger J, 127
 Fukushima T, 118
 Fulop L, 51

Gärtner M, 89
 Gößler M, 39
 Gali A, 44
 Gammer C, 38
 Ganser C, 40
 García-López V, 90
 Garratt Th, 44
 Gas K, 47
 Gatchell M, 103
 Gavalas I, 45
 Geerts Y, 96
 Geltenbort P, 111
 Genes C, 25
 Genser J, 125
 Glatzel T, 102
 Goulart M, 103
 Gründlinger P, 92
 Grünewald M, 127
 Gradwohl K-P, 118
 Graus M, 126
 Greco F, 117, 131
 Grill L, 90–92, 122, 124
 Grimm M, 126
 Grogger W, 110
 Groves C, 128
 Györök M, 92, 123

Hörmann L, 130
 Höfling S, 34, 36
 Hörmann L, 85, 86
 Hüsing N, 46, 119
 Haberfehlner G, 109
 Hagen C, 24
 Hahn H, 16
 Hahn T, 35
 Haider R, 45
 Haidinger L, 93
 Hanghofer I, 106
 Hanus V, 51
 Hasegawa Y, 57
 Haslhofer M, 43, 110
 Hauser A, 82
 Hauser A W, 27, 82, 101
 Hauser R, 99
 Hecht S, 124
 Hedgeland H, 90
 Heering P, 15
 Heim P, 26, 29–31
 Heldand K, 41
 Hengge E, 39
 Herrmann H, 87

Hillbrand J, 33, 36
 Hinger V, 60
 Hinkov B, 34
 Hinterseer S, 23
 Hirn U, 40
 Hirtl A, 56, 113
 Hofer F, 82, 83
 Hofmann F, 127
 Hofmann O T, 85, 86, 108, 130
 Hofmann P, 78
 Hohenester U, 52
 Hollerer M, 84, 86, 87, 126, 133
 Holzbauer M, 34
 Holzinger R, 31, 102
 Hornberger K, 29
 Hotter C, 104
 Huber M Q, 62, 64, 70
 Hurdax P, 84, 128

 Ishiwwari F, 118
 Ivady V, 44
 Ivanov A N, 111, 112

 Jacobson P, 122
 Jacquet M J, 25
 Jaekel S, 124
 Jakiela R, 47
 Jeindl A, 85, 86, 130
 Jenke T, 111
 Jericha E, 112
 Jernej I, 24
 Jones A O F, 96

 Kühnle A, 124
 Kain S, 114
 Kainz M A, 34
 Kainz P, 73
 Kalbitzer H R, 76
 Kaltenegger M, 95
 Kamencek T, 105, 106
 Kamperidis Ch, 51
 Kangaparambil S, 51
 Kaseß C, 23
 Kastner S, 69
 Kaufmann B, 96
 Kawai S, 102
 Kern C S, 124
 Kern W, 64
 Kisiel M, 102
 Kitzler M, 51
 Kleber S, 136
 Kleinsasser W, 30, 31

 Klimin S, 35
 Klinowaja J, 102
 Klopf M, 112
 Knötig H, 34
 Knez D, 82, 83
 Knobloch C, 29
 Koch M, 26, 29–31
 Koch R, 93
 Koeth J, 34
 Koller G, 86, 87
 Kollmann B, 84
 Kollotzek S, 133
 Korn G, 53
 Kotakoski J, 28
 Kothleitner G, 109
 Kovalenko M V, 46
 Kozak W, 75
 Krabberger G J, 44, 108
 Kralj M, 116
 Krammer M, 89, 128
 Kranabetter L, 103, 105
 Kranebetter L, 104
 Kratzer M, 89, 116, 118, 122, 125
 Krausz F, 18
 Kreil D, 42, 43, 110
 Krenn H, 39, 68
 Krenn J R, 52
 Krikun G, 96
 Krok F, 89
 Kuchar F, 54
 Kuhn M, 103
 Kulkarni S, 58
 Kutschera W, 66

 Lüftner D, 84, 86, 87, 124–126
 Lührs L, 39
 Lackner F, 32, 82, 83
 Lackner P, 80
 Laimer F, 103–105
 Lammegger R, 24
 Lammer J, 110
 Larimian S, 51
 Lasserus M, 32, 82, 83
 Lechner R T, 46
 Leising G, 117
 Leitner M, 135
 Leitner T, 136
 Lemmel H, 57
 Leoni T, 123
 Lessa A, 58
 Li T, 47

Lin G, 125
 Lindner R, 124
 Liu D, 122
 Lohner K, 72
 Loss D, 102
 Ludescher L, 46

 M. Kovařík M, 118
 Müllegger S, 93
 MacFarland D, 34
 Madlener T, 57
 Magnes W, 24
 Makurat S, 75
 Malcioğlu O B, 88
 Mapelli M, 16
 Marmioli B, 45, 49
 Martini P, 103
 Marx L, 72, 73
 Matković A, 89, 116, 122, 125
 Matolin V, 115
 Matteucci M, 45
 Matzer M, 47
 Mayr S, 80
 Mayrhofer C, 108
 Mayrhofer-Reinhartshuber M, 73
 Meißner R, 75
 Meier T, 102
 Meisels R, 54
 Messner R, 32, 82, 83
 Metzger C, 126
 Meyer B, 77
 Meyer E, 102
 Meyer M, 29–31
 Meyer R, 27, 82, 101
 Mezger M, 93
 Micko J, 111
 Miramontes A, 65
 Miramontes A S, 65
 Mocnik K, 69
 Mohammadi M, 121
 Monkowius U, 92
 Morak R, 46
 Moser S, 74
 Mueller M J, 99
 Muralter F, 94
 Musso M, 48, 106, 107, 114, 119, 120
 Mysliveček J, 115

 Nacci C, 92
 Nachtnebel M, 108
 Nanda A, 27

 Nascimbeni G, 118
 Navarro-Quezada A, 47, 123
 Netzer F P, 120, 121, 132

 Obersteiner V, 123
 Opacak N, 33, 34
 Ostermann L, 25, 31, 102, 104
 Osvay K, 51
 Otto F, 124

 Pölt P, 37, 83
 Pötz W, 42, 61
 Pápa Z, 52
 Pabst G, 72, 73
 Pachmajer S, 86
 Paischer S, 43
 Papp C, 77
 París-López J, 63
 Paris O, 46
 Pauly S, 38
 Pawlak R, 102
 Perrotta A, 79, 80, 94
 Petricca, 17
 Petritz A, 89
 Petutschnigg A, 114
 Pfleger A J, 70
 Pichler P, 135
 Pilz J, 79, 80
 Pitschmann M, 111
 Plank H, 109, 134
 Plankensteiner D, 31, 102, 104
 Pollastri S, 115
 Pollinger A, 24
 Pomp S, 126
 Postler J, 103
 Pototschnig J V, 32
 Pottlacher G, 20, 135, 136
 Pree E, 60
 Pusching P, 125
 Puschnig P, 84, 86, 87, 124, 126, 127
 Pusterhofer M, 78
 Putz F, 46

 Röthel C, 96
 Rácz P, 52
 Radlinger T, 120
 Rak J, 75
 Ramsey M, 127, 128
 Ramsey M G, 84, 86, 87
 Ranguis A, 123
 Rastogi M, 104
 Raubitzek S, 63

Rauch S, 110
 Rechberger T, 111
 Redinger J, 133
 Reichenauer G, 46
 Reichl Ch, 22
 Reinert F, 126
 Reinisch E-M, 86
 Rentenberger C, 38
 Resel R, 96, 127
 Rettenwander D, 106
 Reyer A, 48, 106, 107, 114, 119, 120
 Richter A, 124
 Ritsch H, 25, 31, 102, 104
 Ritsch-Marte M, 74
 Roncin P, 28
 Rossi B, 48, 107
 Ruckhofer A, 78
 Rumetshofer M, 26
 Russ T, 65
 Ruzie C, 96

 Saßnick H, 44
 Sabathi G, 119
 Sabik A, 90
 Sacher J, 98
 Sachslehner F, 67
 Saller M, 36
 Sanchis-Alepuz H, 62, 63, 65
 Sansone G, 51
 Sartori B, 49
 Sattelkow J, 134
 Sawicki M, 47
 Schönhuber S, 34
 Schütz F, 44
 Schade A, 36
 Scheier P, 103–105, 133
 Scherbela M, 85, 86, 130
 Schider G, 89
 Schied M, 122
 Schiffman A, 82
 Schiffmann A, 32, 82, 83
 Schindl R, 73
 Schlemmer W, 134
 Schmid M, 77, 80, 131
 Schmidt R, 108
 Schmuck K, 101
 Schnedlitz M, 32, 82, 83
 Schneider J, 87
 Schober M, 42
 Schober R, 73
 Scholl A, 126

 Schrenk W, 34
 Schrode B, 95, 127
 Schroettner H, 108
 Schuh D, 111
 Schuster J, 93
 Schwarz B, 33, 36
 Schwarz F, 126
 Schwendt M, 42, 126
 Sedmik R, 111
 Seewald L M, 105, 106
 Seidel P, 126
 Semeraro E F, 72, 73
 Sepperer T, 48, 107
 Shayeghi A, 29
 Sihver L, 56, 113
 Simpson G J, 90, 91
 Siri O, 122, 125
 Sojka F, 127
 Sorantin M, 41
 Spirk S, 134
 Sponar S, 57
 Spreitzer H, 96
 Sprengel W, 39
 Stöllinger P, 65
 Stadlober B, 89
 Steiner D, 133
 Steinrück H-P, 15
 Sterrer M, 81, 84, 86, 87, 126, 128, 133
 Stetsovyeh V, 93
 Steyskal E, 37
 Steyskal E-M, 39
 Stickler B A, 29
 Stoellinger B, 65
 Strahlberg M, 56
 Strasser F, 74
 Strasser G, 14, 33, 34, 36
 Stratakis E, 45
 Surnev S, 120, 121, 132
 Susi T, 28
 Szajna K, 89
 Szedlak R, 34

 Tüchler M, 61
 Taboryski R, 45
 Tamtögl A, 78, 90
 Tanaka K A, 53
 Taucher T C, 123
 Teichert C, 40, 89, 96, 116, 118, 122, 125
 Tempere J, 35
 Terfort A, 89
 Thaler B, 26, 29–31

Thalhammer G, 74
 Thalhammer M, 111
 Thomas A, 123
 Thurner C W, 133
 Tiefenthaler L, 104, 105
 Tondi G, 48, 107, 120
 Tour J M, 90, 122
 Trügler A, 70
 Treiber L, 30, 31
 Tripl C, 60
 Tromba G, 48, 107
 Trummer C, 109

 Udhardt C, 124
 Ulrich-Pur F, 56, 113
 Unterrainer K, 34
 Unzog M, 127

 Vaccari L, 48, 107, 120
 Vaclavu M, 115
 Valentan M, 59, 60
 Valtiner M, 93
 Varju K, 51
 von der Linden W, 26
 von Wrochem F, 118
 Vukušić A, 116

 Würschum R, 37, 39
 Wagner M, 77
 Wagner T, 92, 123
 Ward D J, 90
 Waubke H, 23
 Weber S, 53
 Weih R, 34
 Weinhart P-F, 67
 Weiss H, 93
 Weissmüller J, 39
 Wendisch F, 36
 Wendisch J F, 120
 Werl M, 70
 Werzer O, 95
 Wilkening M, 106
 Wimberger P, 22
 Winkler C, 108
 Winkler D, 20
 Winkler R, 109
 Wolf M, 45, 76
 Wolfmayr S, 92
 Wongel A, 58
 Wrana D, 89

 Xia B, 118

 Xie X, 51
 Xu Y, 118

 Zajki-Zechmeister K, 134
 Zamborlini G, 84
 Zankel A, 108
 Zeppenfeld P, 92, 123
 Zhang B, 118
 Zharnikov M, 118
 Zingl M, 44
 Zojer E, 41, 89, 105, 106, 108, 118, 123
 Zojer K, 89, 96, 128
 Zou Z, 80



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